3-Methyldiphenylmethane

Other names: Diphenylmethane, 3-methyl
Inchi: InChI=1S/C14H14/c1-12-6-5-9-14(10-12)11-13-7-3-2-4-8-13/h2-10H,11H2,1H3
InchiKey: KSYQGOYOIKQFNA-UHFFFAOYSA-N
Formula: C14H14
SMILES: Cc1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]: 182.27
CAS: 620-47-3

Physical Properties

Property code	Value	Unit	Source
af	0.4434		Cheméo Relay (1.0)
chl	-7322.00	kJ/mol	NIST Webbook
gf	282.19	kJ/mol	Joback Method
hf	150.93	kJ/mol	Cheméo Relay (1.0)
hfus	19.71	kJ/mol	Joback Method
hvap	73.26	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-4.58		Cheméo Relay (1.0)
logp	3.586		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1565.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2168.00		NIST Webbook
tb	552.39 ± 0.40	K	NIST Webbook
tb	552.39 ± 0.30	K	NIST Webbook
tb	552.39 ± 0.40	K	NIST Webbook
tc	781.32	K	Cheméo Relay (1.0)
tf	245.32 ± 0.05	K	NIST Webbook
tf	245.32 ± 0.05	K	NIST Webbook
vc	0.612	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.14	J/mol×K	578.06	Joback Method
cpg	389.56	J/mol×K	618.17	Joback Method
cpg	405.71	J/mol×K	658.28	Joback Method
cpg	420.65	J/mol×K	698.39	Joback Method
cpg	434.45	J/mol×K	738.50	Joback Method
cpg	447.19	J/mol×K	778.61	Joback Method
cpg	458.94	J/mol×K	818.72	Joback Method
dvisc	0.0019467	Pa×s	312.90	Joback Method
dvisc	0.0010159	Pa×s	357.09	Joback Method
dvisc	0.0006118	Pa×s	401.29	Joback Method
dvisc	0.0004075	Pa×s	445.48	Joback Method
dvisc	0.0002920	Pa×s	489.67	Joback Method
dvisc	0.0002212	Pa×s	533.87	Joback Method
dvisc	0.0001748	Pa×s	578.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45709e+01
Coeff. B	-4.62981e+03
Coeff. C	-8.72050e+01
Temperature range (K), min.	411.35
Temperature range (K), max.	587.21

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620473&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume