2,4,6-trimethyldodecane

Inchi: InChI=1S/C15H32/c1-6-7-8-9-10-14(4)12-15(5)11-13(2)3/h13-15H,6-12H2,1-5H3
InchiKey: JLQUHHQIHZZTEZ-UHFFFAOYSA-N
Formula: C15H32
SMILES: CCCCCCC(C)CC(C)CC(C)C
Mol. weight [g/mol]: 212.42
CAS: 103387-11-7

Physical Properties

Property code	Value	Unit	Source
af	0.5748		Cheméo Relay (1.0)
gf	68.10	kJ/mol	Joback Method
hf	-390.57	kJ/mol	Cheméo Relay (1.0)
hfus	24.04	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Cheméo Relay (1.0)
ie	9.49	eV	Cheméo Relay (1.0)
log10ws	-7.09		Cheméo Relay (1.0)
logp	5.665		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
tb	510.98	K	Cheméo Relay (1.0)
tc	669.87	K	Cheméo Relay (1.0)
tf	207.14	K	Cheméo Relay (1.0)
vc	0.831	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.60	J/mol×K	541.28	Joback Method
cpg	665.77	J/mol×K	708.78	Joback Method
cpg	649.78	J/mol×K	680.87	Joback Method
cpg	633.08	J/mol×K	652.95	Joback Method
cpg	615.63	J/mol×K	625.03	Joback Method
cpg	597.41	J/mol×K	597.11	Joback Method
cpg	578.41	J/mol×K	569.20	Joback Method

dvisc	0.0006072	Pa×s	377.54	Joback Method
dvisc	0.0001394	Pa×s	541.28	Joback Method
dvisc	0.0002040	Pa×s	486.70	Joback Method
dvisc	0.0003285	Pa×s	432.12	Joback Method
dvisc	0.0251735	Pa×s	213.81	Joback Method
dvisc	0.0013813	Pa×s	322.97	Joback Method
dvisc	0.0043898	Pa×s	268.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78158e+01
Coeff. B	-6.70102e+03
Coeff. C	-4.20000e-01
Temperature range (K), min.	382.72
Temperature range (K), max.	536.32

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume