2-Methylheptacosane

Inchi: InChI=1S/C28H58/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: NIYAMIIVLUIWBI-UHFFFAOYSA-N
Formula: C28H58
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 394.76
CAS: 1561-00-8

Physical Properties

Property code	Value	Unit	Source
gf	182.44	kJ/mol	Joback Method
hf	-626.53	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	11.025		Crippen Method
mcvol	405.380	ml/mol	McGowan Method
pc	658.14	kPa	Joback Method
rinpol	2765.30		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2765.30		NIST Webbook
rinpol	2761.90		NIST Webbook
tb	839.60	K	Joback Method
tc	1029.02	K	Joback Method
tf	390.32	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.23	J/mol×K	1029.02	Joback Method
cpg	1462.81	J/mol×K	997.45	Joback Method
cpg	1442.31	J/mol×K	965.88	Joback Method

cpg	1420.68	J/mol×K	934.31	Joback Method
cpg	1397.85	J/mol×K	902.74	Joback Method
cpg	1373.75	J/mol×K	871.17	Joback Method
cpg	1348.34	J/mol×K	839.60	Joback Method
dvisc	0.0017949	Pa×s	390.32	Joback Method
dvisc	0.0000300	Pa×s	839.60	Joback Method
dvisc	0.0000425	Pa×s	764.72	Joback Method
dvisc	0.0000649	Pa×s	689.84	Joback Method
dvisc	0.0001099	Pa×s	614.96	Joback Method
dvisc	0.0002154	Pa×s	540.08	Joback Method
dvisc	0.0005242	Pa×s	465.20	Joback Method
hvapt	111.90	kJ/mol	574.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47686e+01
Coeff. B	-5.37400e+03
Coeff. C	-1.70450e+02
Temperature range (K), min.	541.56
Temperature range (K), max.	738.70

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1561008&Units=SI

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

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

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

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

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

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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