Pentadecane, 3,7,11-trimethyl

Inchi: InChI=1S/C18H38/c1-6-8-11-17(4)14-10-15-18(5)13-9-12-16(3)7-2/h16-18H,6-15H2,1-5H
InchiKey: DQIDCRGJXXCOMF-UHFFFAOYSA-N
Formula: C18H38
SMILES: CCCCC(C)CCCC(C)CCCC(C)CC
Mol. weight [g/mol]: 254.49

Physical Properties

Property code	Value	Unit	Source
gf	93.36	kJ/mol	Joback Method
hf	-430.69	kJ/mol	Joback Method
hfus	31.81	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.835		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	609.92	K	Joback Method
tc	775.39	K	Joback Method
tf	247.62	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.35	J/mol×K	609.92	Joback Method
cpg	821.01	J/mol×K	747.81	Joback Method
cpg	803.34	J/mol×K	720.23	Joback Method
cpg	784.86	J/mol×K	692.65	Joback Method
cpg	765.56	J/mol×K	665.08	Joback Method
cpg	745.40	J/mol×K	637.50	Joback Method

cpg	837.89	J/mol×K	775.39	Joback Method
dvisc	0.0000998	Pa×s	609.92	Joback Method
dvisc	0.0001461	Pa×s	549.54	Joback Method
dvisc	0.0002352	Pa×s	489.15	Joback Method
dvisc	0.0004328	Pa×s	428.77	Joback Method
dvisc	0.0009729	Pa×s	368.39	Joback Method
dvisc	0.0030046	Pa×s	308.00	Joback Method
dvisc	0.0160811	Pa×s	247.62	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R12177&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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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