

4,5,13-trimethylheptadecane

Inchi: InChI=1S/C20H42/c1-6-8-15-18(3)16-12-10-9-11-13-17-20(5)19(4)14-7-2/h18-20H,6-17H
InchiKey: MARJLHGTVVAEQY-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCC(C)CCCCCCCC(C)C(C)CCC
Mol. weight [g/mol]: 282.55

Physical Properties

Property code	Value	Unit	Source
gf	110.20	kJ/mol	Joback Method
hf	-471.97	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.616		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	1884.00		NIST Webbook
tb	655.68	K	Joback Method
tc	821.33	K	Joback Method
tf	270.16	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.48	J/mol×K	655.68	Joback Method
cpg	941.05	J/mol×K	793.73	Joback Method
cpg	922.89	J/mol×K	766.12	Joback Method
cpg	903.88	J/mol×K	738.51	Joback Method
cpg	883.99	J/mol×K	710.90	Joback Method
cpg	863.20	J/mol×K	683.29	Joback Method
cpg	958.39	J/mol×K	821.33	Joback Method
dvisc	0.0000778	Pa×s	655.68	Joback Method
dvisc	0.0001140	Pa×s	591.43	Joback Method

dvisc	0.0001834	Pa×s	527.17	Joback Method
dvisc	0.0003367	Pa×s	462.92	Joback Method
dvisc	0.0007518	Pa×s	398.67	Joback Method
dvisc	0.0022855	Pa×s	334.41	Joback Method
dvisc	0.0117916	Pa×s	270.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273655&Units=SI
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

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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