

4,12,13-trimethylheptadecane

Inchi:	InChI=1S/C20H42/c1-6-8-16-19(4)20(5)17-13-11-9-10-12-15-18(3)14-7-2/h18-20H,6-17H
InchiKey:	NLCWCYCSPFIIGT-UHFFFAOYSA-N
Formula:	C20H42
SMILES:	CCCC(C)C(C)CCCCCCC(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
mvol	292.660	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	1879.00		NIST Webbook
tb	655.68	K	Joback Method
tc	821.33	K	Joback Method
tf	270.16	K	Joback Method
vc	1.137	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.48	J/mol×K	655.68	Joback Method
cpg	863.20	J/mol×K	683.29	Joback Method
cpg	883.99	J/mol×K	710.90	Joback Method
cpg	903.88	J/mol×K	738.51	Joback Method
cpg	922.89	J/mol×K	766.12	Joback Method
cpg	941.05	J/mol×K	793.73	Joback Method
cpg	958.39	J/mol×K	821.33	Joback Method
dvisc	0.0117916	Paxs	270.16	Joback Method
dvisc	0.0022855	Paxs	334.41	Joback Method

dvisc	0.0007518	Paxs	398.67	Joback Method
dvisc	0.0003367	Paxs	462.92	Joback Method
dvisc	0.0001834	Paxs	527.17	Joback Method
dvisc	0.0001140	Paxs	591.43	Joback Method
dvisc	0.0000778	Paxs	655.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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