

Hexadecane, 2,6,11,15-tetramethyl-

Other names:	Crocetane 2,6,11,15-Tetramethylhexadecane
Inchi:	InChI=1S/C20H42/c1-17(2)11-9-15-19(5)13-7-8-14-20(6)16-10-12-18(3)4/h17-20H,7-16H
InchiKey:	KKFZXXATNGJPJS-UHFFFAOYSA-N
Formula:	C20H42
SMILES:	CC(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	282.55
CAS:	504-44-9

Physical Properties

Property code	Value	Unit	Source
gf	107.76	kJ/mol	Joback Method
hf	-477.25	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	58.56	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	7.472		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1792.00		NIST Webbook
tb	592.00 ± 0.60	K	NIST Webbook
tc	822.89	K	Joback Method
tf	255.16	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.81	J/mol×K	655.24	Joback Method
cpg	863.83	J/mol×K	683.18	Joback Method
cpg	884.89	J/mol×K	711.12	Joback Method
cpg	905.01	J/mol×K	739.06	Joback Method

cpg	924.24	J/molxK	767.00	Joback Method
cpg	942.58	J/molxK	794.94	Joback Method
cpg	960.09	J/molxK	822.89	Joback Method
dvisc	0.0197594	Paxs	255.16	Joback Method
dvisc	0.0029435	Paxs	321.84	Joback Method
dvisc	0.0008429	Paxs	388.52	Joback Method
dvisc	0.0003482	Paxs	455.20	Joback Method
dvisc	0.0001803	Paxs	521.88	Joback Method
dvisc	0.0001084	Paxs	588.56	Joback Method
dvisc	0.0000722	Paxs	655.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504449&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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