Cyprotene

Inchi:	InChI=1S/C14H24/c1-6-11-9-12-8-7-10(2)14(11,5)13(12,3)4/h6,10,12H,7-9H2,1-5H3/b11
InchiKey:	FMOZOFOCONBPNY-RAYWUTBOSA-N
Formula:	C14H24
SMILES:	CC=C1CC2CCC(C)C1(C)C2(C)C
Mol. weight [g/mol]:	192.34
CAS:	193695-14-6

Physical Properties

Property code	Value	Unit	Source
gf	183.36	kJ/mol	Joback Method
hf	-133.18	kJ/mol	Joback Method
hfus	13.95	kJ/mol	Joback Method
hvap	44.80	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.415		Crippen Method
mcvol	182.100	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1327.00		NIST Webbook
tb	539.52	K	Joback Method
tc	756.56	K	Joback Method
tf	326.06	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.63	J/mol×K	539.52	Joback Method
cpg	487.66	J/mol×K	575.69	Joback Method
cpg	508.21	J/mol×K	611.87	Joback Method
cpg	527.51	J/mol×K	648.04	Joback Method

cpg	545.80	J/mol×K	684.21	Joback Method
cpg	563.32	J/mol×K	720.39	Joback Method
cpg	580.30	J/mol×K	756.56	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=C193695146&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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