Pregeijerene B

Inchi: InChI=1S/C12H18/c1-11-7-4-3-5-8-12(2)10-6-9-11/h3-4,8-9H,5-7,10H2,1-2H3/b4-3-,11-9
InchiKey: HJFJPKDXNZHKGG-DZTLHLKESA-N
Formula: C12H18
SMILES: CC1=CCCC(C)=CCC=CC1
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	104.54	kJ/mol	Joback Method
hf	-90.59	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.009		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1503.00		NIST Webbook
tb	522.70	K	Joback Method
tc	755.05	K	Joback Method
tf	249.86	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.81	J/mol×K	522.70	Joback Method
cpg	368.58	J/mol×K	561.43	Joback Method
cpg	388.19	J/mol×K	600.15	Joback Method
cpg	406.64	J/mol×K	638.88	Joback Method

cpg	423.95	J/mol×K	677.60	Joback Method
cpg	440.11	J/mol×K	716.33	Joback Method
cpg	455.13	J/mol×K	755.05	Joback Method
dvisc	0.0098765	Pa×s	249.86	Joback Method
dvisc	0.0024293	Pa×s	295.33	Joback Method
dvisc	0.0008688	Pa×s	340.81	Joback Method
dvisc	0.0003958	Pa×s	386.28	Joback Method
dvisc	0.0002128	Pa×s	431.75	Joback Method
dvisc	0.0001288	Pa×s	477.23	Joback Method
dvisc	0.0000850	Pa×s	522.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419628&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume