Seyschellene

Inchi: InChI=1S/C16H26/c1-7-15(5)14-10-12(3)13(4)16(15,6)9-8-11(14)2/h10-12H,4,7-9H2,1-3
InchiKey: JPLQRSHDQYTTIH-FTYWFFQTSA-N
Formula: C16H26
SMILES: C=C1C(C)C=C2C(C)CCC1(C)C2(C)CC
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
gf	216.05	kJ/mol	Joback Method
hf	-126.10	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.971		Crippen Method
mcvol	205.980	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	586.21	K	Joback Method
tc	801.46	K	Joback Method
tf	361.68	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.16	J/mol×K	586.21	Joback Method
cpg	572.21	J/mol×K	622.09	Joback Method
cpg	593.03	J/mol×K	657.96	Joback Method
cpg	612.83	J/mol×K	693.84	Joback Method
cpg	631.84	J/mol×K	729.71	Joback Method
cpg	650.26	J/mol×K	765.59	Joback Method
cpg	668.31	J/mol×K	801.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R625393&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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