trans-Methylisocosticate

Inchi: InChI=1S/C16H24O2/c1-11-6-5-8-16(3)9-7-13(10-14(11)16)12(2)15(17)18-4/h13H,2,5-10
InchiKey: OWZSHJKGKHTKDS-BBRMVZONSA-N
Formula: C16H24O2
SMILES: C=C(C(=O)OC)C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]: 248.36
CAS: 132342-55-3

Physical Properties

Property code	Value	Unit	Source
gf	7.52	kJ/mol	Joback Method
hf	-331.69	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.022		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1791.90		NIST Webbook
rinpol	1791.90		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	678.25	K	Joback Method
tc	903.67	K	Joback Method
tf	398.02	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.26	J/mol×K	678.25	Joback Method
cpg	629.72	J/mol×K	715.82	Joback Method
cpg	649.10	J/mol×K	753.39	Joback Method
cpg	667.55	J/mol×K	790.96	Joback Method
cpg	685.22	J/mol×K	828.53	Joback Method
cpg	702.26	J/mol×K	866.10	Joback Method

cpg	718.81	J/mol×K	903.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132342553&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
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