Acetic acid, 2-cyano-2-[1-methyl-4-(1,1-dimethylethyl)cyclohex ethyl ester, #1

Inchi: InChI=1S/C16H27NO2/c1-6-19-14(18)13(11-17)16(5)9-7-12(8-10-16)15(2,3)4/h12-13H,6
InchiKey: YIKKFVFXWIZXKG-UHFFFAOYSA-N
Formula: C16H27NO2
SMILES: CCOC(=O)C(C#N)C1(C)CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 265.39

Physical Properties

Property code	Value	Unit	Source
gf	-5.25	kJ/mol	Joback Method
hf	-418.30	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	68.13	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.932		Crippen Method
mcvol	234.260	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1743.00		NIST Webbook
ripol	2166.00		NIST Webbook
ripol	2166.00		NIST Webbook
tb	755.30	K	Joback Method
tc	977.05	K	Joback Method
tf	421.69	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.00	J/mol×K	755.30	Joback Method
cpg	735.09	J/mol×K	792.26	Joback Method
cpg	753.30	J/mol×K	829.22	Joback Method
cpg	770.75	J/mol×K	866.17	Joback Method

cpg	787.60	J/mol×K	903.13	Joback Method
cpg	803.96	J/mol×K	940.09	Joback Method
cpg	820.00	J/mol×K	977.05	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=R97684&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume