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

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	1781.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1781.00		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:	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=R97698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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