

Tricyclo[3.3.1.13,7]decane-2-acetic acid, «alpha»-cyano-ethyl ester

Other names:	Adamantaneacetic acid, «delta»-[2(«alpha»)]-«alpha»-cyano-, ethyl ester
Inchi:	InChI=1S/C15H21NO2/c1-2-18-15(17)13(8-16)14-11-4-9-3-10(6-11)7-12(14)5-9/h9-14H,
InchiKey:	NKQDZOMRNC AJHD-UHFFFAOYSA-N
Formula:	C15H21NO2
SMILES:	CCOC(=O)C(C#N)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	247.33
CAS:	52567-21-2

Physical Properties

Property code	Value	Unit	Source
gf	126.97	kJ/mol	Joback Method
hf	-266.57	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.762		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
tb	735.68	K	Joback Method
tc	956.16	K	Joback Method
tf	422.78	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.66	J/mol×K	735.68	Joback Method
cpg	645.22	J/mol×K	772.43	Joback Method
cpg	661.64	J/mol×K	809.17	Joback Method
cpg	677.01	J/mol×K	845.92	Joback Method
cpg	691.41	J/mol×K	882.67	Joback Method
cpg	704.95	J/mol×K	919.41	Joback Method
cpg	717.71	J/mol×K	956.16	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=C52567212&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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