

Ethyladamantane-1-carboxylate

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-carboxylic acid, ethyl ester ethyl tricyclo[3.3.1.13,7]decane-1-carboxylate
Inchi:	InChI=1S/C13H20O2/c1-2-15-12(14)13-6-9-3-10(7-13)5-11(4-9)8-13/h9-11H,2-8H2,1H3
InchiKey:	SYEXGNJRYPOUSI-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CCOC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	208.30
CAS:	2094-73-7

Physical Properties

Property code	Value	Unit	Source
gf	-18.39	kJ/mol	Joback Method
hf	-349.31	kJ/mol	Joback Method
hfus	19.29	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.766		Crippen Method
mcvol	168.890	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1917.00		NIST Webbook
tb	593.19	K	Joback Method
tc	812.11	K	Joback Method
tf	378.39	K	Joback Method
vc	0.647	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.08	J/mol×K	593.19	Joback Method
cpg	494.67	J/mol×K	629.68	Joback Method
cpg	513.00	J/mol×K	666.16	Joback Method
cpg	530.22	J/mol×K	702.65	Joback Method
cpg	546.54	J/mol×K	739.14	Joback Method
cpg	562.12	J/mol×K	775.62	Joback Method
cpg	577.14	J/mol×K	812.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.00	K	1.00	NIST Webbook

Sources

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=C2094737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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