

Esprocarb

Other names:	Carbamothioic acid, N-(1,2-dimethylpropyl)-N-ethyl-, S-(phenylmethyl) ester
Inchi:	InChI=1S/C15H23NOS/c1-5-16(13(4)12(2)3)15(17)18-11-14-9-7-6-8-10-14/h6-10,12-13H
InchiKey:	BXEHUCNTIZGSOJ-UHFFFAOYSA-N
Formula:	C15H23NOS
SMILES:	CCN(C(=O)SCc1ccccc1)C(C)C(C)C
Mol. weight [g/mol]:	265.41
CAS:	85785-20-2

Physical Properties

Property code	Value	Unit	Source
gf	197.93	kJ/mol	Joback Method
hf	-130.14	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.406		Crippen Method
mcvol	226.350	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	703.49	K	Joback Method
tc	922.81	K	Joback Method
tf	372.03	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.57	J/molxK	703.49	Joback Method
cpg	637.03	J/molxK	740.04	Joback Method
cpg	653.27	J/molxK	776.60	Joback Method
cpg	668.35	J/molxK	813.15	Joback Method

cpg	682.33	J/mol×K	849.71	Joback Method
cpg	695.26	J/mol×K	886.26	Joback Method
cpg	707.19	J/mol×K	922.81	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=C85785202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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