

Ethomoxane

Other names:	(.+/-)-2-(Butylaminomethyl)-8-ethoxy-1,4-benzodioxan
Inchi:	InChI=1S/C15H23NO3/c1-3-5-9-16-10-12-11-18-14-8-6-7-13(17-4-2)15(14)19-12/h6-8,1
InchiKey:	WKRAEDUMAWVCOG-UHFFFAOYSA-N
Formula:	C15H23NO3
SMILES:	CCCCNCC1COc2cccc(OCC)c2O1
Mol. weight [g/mol]:	265.35
CAS:	16509-23-2

Physical Properties

Property code	Value	Unit	Source
gf	29.37	kJ/mol	Joback Method
hf	-415.45	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	70.53	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.615		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	716.74	K	Joback Method
tc	924.70	K	Joback Method
tf	452.72	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.50	J/molxK	716.74	Joback Method
cpg	651.42	J/molxK	751.40	Joback Method
cpg	667.29	J/molxK	786.06	Joback Method
cpg	682.17	J/molxK	820.72	Joback Method
cpg	696.08	J/molxK	855.38	Joback Method
cpg	709.06	J/molxK	890.04	Joback Method

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=C16509232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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