

3-(2-Ethylhexoxy)propan-1-amine, N-acetate

Other names:	1-Propanamine, 3-[(2-ethylhexyl)oxy]-, N-acetate 3-(2-Ethylhexyloxy)-propylamine, N-acetate 2-Ethylhexyl 3-acetaminopropyl ether 3-(2-Ethylhexoxy)propylamine, N-acetate
Inchi:	InChI=1S/C13H27NO2/c1-4-6-8-13(5-2)11-16-10-7-9-14-12(3)15/h13H,4-11H2,1-3H3,(H
InchiKey:	JROXMRVYNAHIMS-UHFFFAOYSA-N
Formula:	C13H27NO2
SMILES:	CCCCC(CC)COCCNC(C)=O
Mol. weight [g/mol]:	229.36

Physical Properties

Property code	Value	Unit	Source
gf	-88.39	kJ/mol	Joback Method
hf	-508.26	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.746		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinsol	1735.00		NIST Webbook
tb	622.86	K	Joback Method
tc	797.16	K	Joback Method
tf	346.09	K	Joback Method
vc	0.817	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.77	J/mol×K	622.86	Joback Method
cpg	590.24	J/mol×K	651.91	Joback Method
cpg	605.99	J/mol×K	680.96	Joback Method
cpg	621.03	J/mol×K	710.01	Joback Method
cpg	635.37	J/mol×K	739.06	Joback Method

cpg	649.02	J/mol×K	768.11	Joback Method
cpg	662.00	J/mol×K	797.16	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=U378203&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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