N-Acetyl-N-(3-[(2-ethylhexyl)oxy]propyl)acetamide

Other names: 1-Propanamine, 3-[(2-ethylhexyl)oxy]-, N,N-diacetate
2-Ethylhexyl 3-di-acetaminopropyl ether
3-(2-Ethylhexoxy)propan-1-amine, N,N-diacetyl
N-Acetyl-N-{3-[(2-ethylhexyl)oxy]propyl}acetamide
Inchi: InChI=1S/C15H29NO3/c1-5-7-9-15(6-2)12-19-11-8-10-16(13(3)17)14(4)18/h15H,5-12H2
InchiKey: WZCSCPCGOWIXKI-UHFFFAOYSA-N
Formula: C15H29NO3
SMILES: CCCCC(CC)COCCCN(C(C)=O)C(C)=O
Mol. weight [g/mol]: 271.40

Physical Properties

Property code	Value	Unit	Source
gf	-179.08	kJ/mol	Joback Method
hf	-648.06	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	3.004		Crippen Method
mcvol	241.200	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	684.76	K	Joback Method
tc	861.70	K	Joback Method
tf	398.37	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.79	J/mol×K	684.76	Joback Method
cpg	705.58	J/mol×K	714.25	Joback Method
cpg	721.55	J/mol×K	743.74	Joback Method
cpg	736.70	J/mol×K	773.23	Joback Method

cpg	751.06	J/mol×K	802.72	Joback Method
cpg	764.66	J/mol×K	832.21	Joback Method
cpg	777.50	J/mol×K	861.70	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=U373429&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume