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

Other names: 2-Ethylhexyl 3-trifluoroacetaminopropyl ether
N-(3-[(2-Ethylhexyl)oxy]propyl)-2,2,2-trifluoroacetamide

Inchi: InChI=1S/C13H24F3NO2/c1-3-5-7-11(4-2)10-19-9-6-8-17-12(18)13(14,15)16/h11H,3-10

InchiKey: ICTVAXQPDDSLGE-UHFFFAOYSA-N

Formula: C13H24F3NO2

SMILES: CCCCC(CC)COCCCNC(=O)C(F)(F)F

Mol. weight [g/mol]: 283.33

Physical Properties

Property code	Value	Unit	Source
gf	-669.98	kJ/mol	Joback Method
hf	-1105.34	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.288		Crippen Method
mcvol	216.760	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
tb	617.44	K	Joback Method
tc	781.14	K	Joback Method
tf	350.28	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.56	J/mol×K	617.44	Joback Method
cpg	615.86	J/mol×K	644.72	Joback Method
cpg	630.45	J/mol×K	672.01	Joback Method
cpg	644.34	J/mol×K	699.29	Joback Method
cpg	657.55	J/mol×K	726.57	Joback Method
cpg	670.12	J/mol×K	753.86	Joback Method

cpg	682.06	J/mol×K	781.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U373430&Units=SI

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