

3-(2-ETHYLHEXYLOXY)PROPYLAMINE

Other names:	1-Propanamine, 3-[(2-ethylhexyl)oxy]- Propylamine, 3-(2-ethylhexoxy)- Propylamine, 3-((2-ethylhexyl)oxy)- 2-Ethylhexyl 3-aminopropyl ether 3-(2-Ethylhexoxy)propylamine NSC 1078 3-(2-Ethylhexoxy)propan-1-amine
Inchi:	InChI=1S/C11H25NO/c1-3-5-7-11(4-2)10-13-9-6-8-12/h11H,3-10,12H2,1-2H3
InchiKey:	DVFGEIYOLIFSRX-UHFFFAOYSA-N
Formula:	C11H25NO
SMILES:	CCCCC(CC)COCCCN
Mol. weight [g/mol]:	187.33

Physical Properties

Property code	Value	Unit	Source
af	0.6477		Cheméo Relay (1.0)
hf	-382.90	kJ/mol	Cheméo Relay (1.0)
hfus	27.11	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.63		Cheméo Relay (1.0)
logp	2.568		Crippen Method
mcvol	181.700	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
tb	517.97	K	Cheméo Relay (1.0)
tc	684.98	K	Cheméo Relay (1.0)
tf	210.53	K	Cheméo Relay (1.0)
vc	0.641	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.32	J/mol×K	545.59	Joback Method

cpg	474.50	J/mol×K	574.86	Joback Method
cpg	490.03	J/mol×K	604.13	Joback Method
cpg	504.92	J/mol×K	633.40	Joback Method
cpg	519.18	J/mol×K	662.67	Joback Method
cpg	532.82	J/mol×K	691.94	Joback Method
cpg	545.86	J/mol×K	721.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5397319&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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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