Propanamide, N,N-bis(2-ethylhexyl)-2-methyl-

Other names: N,N-di-2-ethylhexylisobutyramide
Inchi: InChI=1S/C20H41NO/c1-7-11-13-18(9-3)15-21(20(22)17(5)6)16-19(10-4)14-12-8-2/h17-1
InchiKey: TYDFWJHDNHXBRF-UHFFFAOYSA-N
Formula: C20H41NO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)C(C)C
Mol. weight [g/mol]: 311.55

Physical Properties

Property code	Value	Unit	Source
gf	92.06	kJ/mol	Joback Method
hf	-517.02	kJ/mol	Joback Method
hfus	79.08	kJ/mol	Enthalpies of vaporization of N,N-dialkyl monamides at 298.15K
hvap	67.74	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.904		Crippen Method
mcvol	304.210	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
tb	721.99	K	Joback Method
tc	895.97	K	Joback Method
tf	352.56	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.74	J/mol×K	721.99	Joback Method
cpg	940.34	J/mol×K	750.99	Joback Method
cpg	959.93	J/mol×K	779.98	Joback Method
cpg	978.56	J/mol×K	808.98	Joback Method
cpg	996.26	J/mol×K	837.97	Joback Method

cpg	1013.07	J/mol×K	866.97	Joback Method
cpg	1029.02	J/mol×K	895.97	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of vaporization of N,N-dialkyl monamides at 298.15K:	https://www.doi.org/10.1016/j.tca.2009.05.007
Determination of Activity Coefficients at Infinite Dilution of Solutes in N,N-Di(2-ethylhexyl)isobutyramide Using Inverse Gas-Liquid Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00635
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=U308084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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