

Pentanamide, N,N-bis(2-ethylhexyl)-

Inchi:	InChI=1S/C21H43NO/c1-6-11-14-19(9-4)17-22(21(23)16-13-8-3)18-20(10-5)15-12-7-2/h
InchiKey:	WKPLQXJHLUWPJN-UHFFFAOYSA-N
Formula:	C21H43NO
SMILES:	CCCCC(=O)N(CC(CC)CCCC)CC(CC)CCCC
Mol. weight [g/mol]:	325.57

Physical Properties

Property code	Value	Unit	Source
gf	102.92	kJ/mol	Joback Method
hf	-532.38	kJ/mol	Joback Method
hfus	47.72	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	6.438		Crippen Method
mcvol	318.300	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinqol	2089.00		NIST Webbook
tb	745.31	K	Joback Method
tc	919.42	K	Joback Method
tf	378.83	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.24	J/mol×K	745.31	Joback Method
cpg	1001.00	J/mol×K	774.33	Joback Method
cpg	1020.74	J/mol×K	803.35	Joback Method
cpg	1039.51	J/mol×K	832.37	Joback Method
cpg	1057.34	J/mol×K	861.39	Joback Method
cpg	1074.28	J/mol×K	890.40	Joback Method
cpg	1090.36	J/mol×K	919.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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