

Benzamide, N,N-bis(2-ethylhexyl)-4-ethyl-

Inchi:	InChI=1S/C25H43NO/c1-6-11-13-22(9-4)19-26(20-23(10-5)14-12-7-2)25(27)24-17-15-21
InchiKey:	QMLQJSKZDBTCFH-UHFFFAOYSA-N
Formula:	C25H43NO
SMILES:	CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	373.62

Physical Properties

Property code	Value	Unit	Source
gf	239.38	kJ/mol	Joback Method
hf	-389.88	kJ/mol	Joback Method
hfus	51.73	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.124		Crippen Method
mvol	350.900	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	868.49	K	Joback Method
tc	1067.23	K	Joback Method
tf	462.85	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.63	J/molxK	868.49	Joback Method
cpg	1162.75	J/molxK	901.61	Joback Method
cpg	1181.67	J/molxK	934.74	Joback Method
cpg	1199.44	J/molxK	967.86	Joback Method
cpg	1216.14	J/molxK	1000.98	Joback Method
cpg	1231.84	J/molxK	1034.10	Joback Method
cpg	1246.61	J/molxK	1067.23	Joback Method

Sources

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=U308547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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