

Benzamide, N,N-bis(2-ethylhexyl)-2,3,4-trifluoro-

Inchi:	InChI=1S/C23H36F3NO/c1-5-9-11-17(7-3)15-27(16-18(8-4)12-10-6-2)23(28)19-13-14-20
InchiKey:	WAVNZCNDZIPKDP-UHFFFAOYSA-N
Formula:	C23H36F3NO
SMILES:	CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]:	399.53

Physical Properties

Property code	Value	Unit	Source
gf	-381.15	kJ/mol	Joback Method
hf	-959.87	kJ/mol	Joback Method
hfus	55.01	kJ/mol	Joback Method
hvap	76.62	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.979		Crippen Method
mcvol	328.030	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	830.50	K	Joback Method
tc	1019.02	K	Joback Method
tf	467.12	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.48	J/mol×K	830.50	Joback Method
cpg	1058.86	J/mol×K	861.92	Joback Method
cpg	1076.17	J/mol×K	893.34	Joback Method
cpg	1092.46	J/mol×K	924.76	Joback Method
cpg	1107.78	J/mol×K	956.18	Joback Method
cpg	1122.17	J/mol×K	987.60	Joback Method
cpg	1135.69	J/mol×K	1019.02	Joback Method

Sources

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=U308422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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