

Benzamide, N,N-bis(2-ethylhexyl)-3-trifluoromethyl-

Inchi: InChI=1S/C24H38F3NO/c1-5-9-12-19(7-3)17-28(18-20(8-4)13-10-6-2)23(29)21-14-11-15

InchiKey: GPFZSNFJPJKEOK-UHFFFAOYSA-N

Formula: C24H38F3NO

SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 413.56

Physical Properties

Property code	Value	Unit	Source
gf	-350.63	kJ/mol	Joback Method
hf	-966.32	kJ/mol	Joback Method
hfus	50.97	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.580		Crippen Method
mcvol	342.120	ml/mol	McGowan Method
pc	949.67	kPa	Joback Method
rinpol	2232.00		NIST Webbook
tb	840.19	K	Joback Method
tc	1031.54	K	Joback Method
tf	455.77	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.69	J/molxK	840.19	Joback Method
cpg	1121.53	J/molxK	872.08	Joback Method
cpg	1139.27	J/molxK	903.97	Joback Method
cpg	1155.97	J/molxK	935.86	Joback Method
cpg	1171.72	J/molxK	967.76	Joback Method
cpg	1186.59	J/molxK	999.65	Joback Method
cpg	1200.66	J/molxK	1031.54	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=U308227&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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