

Benzamide, 2,3,4-trifluoro-N-butyl-N-hexadecyl-

Inchi: InChI=1S/C27H44F3NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-22-31(21-6-4-2)27(32)

InchiKey: XDTCWZUXZDIJEE-UHFFFAOYSA-N

Formula: C27H44F3NO

SMILES: CCCCCCCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 455.64

Physical Properties

Property code	Value	Unit	Source
gf	-342.59	kJ/mol	Joback Method
hf	-1031.87	kJ/mol	Joback Method
hfus	72.42	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	8.828		Crippen Method
mvol	384.390	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	922.90	K	Joback Method
tc	1133.04	K	Joback Method
tf	542.20	K	Joback Method
vc	1.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.34	J/mol×K	922.90	Joback Method
cpg	1309.92	J/mol×K	957.92	Joback Method
cpg	1329.17	J/mol×K	992.95	Joback Method
cpg	1347.19	J/mol×K	1027.97	Joback Method
cpg	1364.04	J/mol×K	1063.00	Joback Method
cpg	1379.80	J/mol×K	1098.02	Joback Method
cpg	1394.56	J/mol×K	1133.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415691&Units=SI

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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