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

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

Physical Properties

Property code	Value	Unit	Source
gf	-397.66	kJ/mol	Joback Method
hf	-963.37	kJ/mol	Joback Method
hfus	64.14	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	7.315		Crippen Method
mcvol	328.030	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	869.11	K	Joback Method
tc	1064.18	K	Joback Method
tf	517.31	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.17	J/mol×K	869.11	Joback Method
cpg	1077.95	J/mol×K	901.62	Joback Method
cpg	1094.66	J/mol×K	934.13	Joback Method
cpg	1110.33	J/mol×K	966.64	Joback Method
cpg	1125.03	J/mol×K	999.16	Joback Method
cpg	1138.78	J/mol×K	1031.67	Joback Method
cpg	1151.65	J/mol×K	1064.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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