Benzamide, N,N-dioctyl-4-trifluoromethyl-

Inchi: InChI=1S/C24H38F3NO/c1-3-5-7-9-11-13-19-28(20-14-12-10-8-6-4-2)23(29)21-15-17-22
InchiKey: TUWHZXSSTFVNPK-UHFFFAOYSA-N
Formula: C24H38F3NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 413.56

Physical Properties

Property code	Value	Unit	Source
gf	-345.75	kJ/mol	Joback Method
hf	-955.76	kJ/mol	Joback Method
hfus	58.01	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	7.869		Crippen Method
mcvol	342.120	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2484.00		NIST Webbook
tb	841.07	K	Joback Method
tc	1031.11	K	Joback Method
tf	485.77	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.75	J/mol×K	841.07	Joback Method
cpg	1120.48	J/mol×K	872.74	Joback Method
cpg	1138.14	J/mol×K	904.42	Joback Method
cpg	1154.79	J/mol×K	936.09	Joback Method
cpg	1170.53	J/mol×K	967.77	Joback Method
cpg	1185.42	J/mol×K	999.44	Joback Method
cpg	1199.53	J/mol×K	1031.11	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=U308254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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