Benzamide, N-heptyl-N-octyl-3-trifluoromethyl-

Inchi: InChI=1S/C23H36F3NO/c1-3-5-7-9-11-13-18-27(17-12-10-8-6-4-2)22(28)20-15-14-16-21
InchiKey: QDQKRUAXSFJYHK-UHFFFAOYSA-N
Formula: C23H36F3NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 399.53

Physical Properties

Property code	Value	Unit	Source
gf	-354.17	kJ/mol	Joback Method
hf	-935.12	kJ/mol	Joback Method
hfus	55.42	kJ/mol	Joback Method
hvap	74.77	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.479		Crippen Method
mcvol	328.030	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	2372.00		NIST Webbook
tb	818.19	K	Joback Method
tc	1005.06	K	Joback Method
tf	474.50	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.60	J/mol×K	818.19	Joback Method
cpg	1058.92	J/mol×K	849.33	Joback Method
cpg	1076.20	J/mol×K	880.48	Joback Method
cpg	1092.51	J/mol×K	911.62	Joback Method
cpg	1107.91	J/mol×K	942.77	Joback Method
cpg	1122.48	J/mol×K	973.91	Joback Method
cpg	1136.28	J/mol×K	1005.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308229&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