Benzamide, 3-trifluoromethyl-2-fluoro-N-octyl-

Inchi: InChI=1S/C16H21F4NO/c1-2-3-4-5-6-7-11-21-15(22)12-9-8-10-13(14(12)17)16(18,19)20
InchiKey: NSCPNSFMFOSFQI-UHFFFAOYSA-N
Formula: C16H21F4NO
SMILES: CCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 319.34

Physical Properties

Property code	Value	Unit	Source
gf	-638.94	kJ/mol	Joback Method
hf	-1012.28	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	63.43	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.935		Crippen Method
mcvol	231.170	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	700.01	K	Joback Method
tc	881.28	K	Joback Method
tf	428.91	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.64	J/mol×K	700.01	Joback Method
cpg	677.32	J/mol×K	730.22	Joback Method
cpg	691.15	J/mol×K	760.43	Joback Method
cpg	704.18	J/mol×K	790.65	Joback Method
cpg	716.45	J/mol×K	820.86	Joback Method
cpg	728.00	J/mol×K	851.07	Joback Method
cpg	738.88	J/mol×K	881.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407708&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
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