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

Inchi: InChI=1S/C15H20F3NO/c1-2-3-4-5-6-7-10-19-15(20)11-8-9-12(16)14(18)13(11)17/h8-9H
InchiKey: QHIUFQNFCDTOMV-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-465.02	kJ/mol	Joback Method
hf	-798.25	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	63.98	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.194		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	686.07	K	Joback Method
tc	867.72	K	Joback Method
tf	427.15	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.60	J/mol×K	686.07	Joback Method
cpg	611.91	J/mol×K	716.34	Joback Method
cpg	625.46	J/mol×K	746.62	Joback Method
cpg	638.30	J/mol×K	776.89	Joback Method
cpg	650.43	J/mol×K	807.17	Joback Method
cpg	661.88	J/mol×K	837.44	Joback Method
cpg	672.67	J/mol×K	867.72	Joback Method

Sources

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=U407267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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