Benzamide, 2-(trifluoromethyl)-N-octyl-

Inchi: InChI=1S/C16H22F3NO/c1-2-3-4-5-6-9-12-20-15(21)13-10-7-8-11-14(13)16(17,18)19/h7
InchiKey: UEHCVFDGBJTKHT-UHFFFAOYSA-N
Formula: C16H22F3NO
SMILES: CCCCCCCCNC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-434.50	kJ/mol	Joback Method
hf	-804.70	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.796		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	695.76	K	Joback Method
tc	881.99	K	Joback Method
tf	415.80	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.29	J/mol×K	695.76	Joback Method
cpg	670.64	J/mol×K	726.80	Joback Method
cpg	685.07	J/mol×K	757.84	Joback Method
cpg	698.64	J/mol×K	788.88	Joback Method
cpg	711.39	J/mol×K	819.91	Joback Method
cpg	723.38	J/mol×K	850.95	Joback Method
cpg	734.65	J/mol×K	881.99	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=U407192&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