Benzamide, 2,5-di(trifluoromethyl)-N-octyl-

Inchi: InChI=1S/C17H21F6NO/c1-2-3-4-5-6-7-10-24-15(25)13-11-12(16(18,19)20)8-9-14(13)17
InchiKey: JOSFATBGLZJFRY-UHFFFAOYSA-N
Formula: C17H21F6NO
SMILES: CCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 369.35

Physical Properties

Property code	Value	Unit	Source
gf	-1017.30	kJ/mol	Joback Method
hf	-1433.89	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.815		Crippen Method
mcvol	248.800	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	718.20	K	Joback Method
tc	895.35	K	Joback Method
tf	443.78	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.51	J/mol×K	718.20	Joback Method
cpg	749.89	J/mol×K	747.73	Joback Method
cpg	763.40	J/mol×K	777.25	Joback Method
cpg	776.11	J/mol×K	806.78	Joback Method
cpg	788.06	J/mol×K	836.30	Joback Method
cpg	799.30	J/mol×K	865.83	Joback Method
cpg	809.90	J/mol×K	895.35	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=U407925&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