Benzamide, 3-trifluoromethyl-N-octadecyl-N-butyl-

Inchi: InChI=1S/C30H50F3NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-34(24-6-4-2
InchiKey: YVXDXIDZBGIONK-UHFFFAOYSA-N
Formula: C30H50F3NO
SMILES: CCCCCCCCCCCCCCCCCCCN(CCCC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 497.72

Physical Properties

Property code	Value	Unit	Source
gf	-295.23	kJ/mol	Joback Method
hf	-1079.60	kJ/mol	Joback Method
hfus	73.55	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-11.09		Crippen Method
logp	10.209		Crippen Method
mcvol	426.660	ml/mol	McGowan Method
pc	679.23	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	978.35	K	Joback Method
tc	1207.23	K	Joback Method
tf	553.39	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.24	J/mol×K	978.35	Joback Method
cpg	1504.79	J/mol×K	1016.50	Joback Method
cpg	1525.96	J/mol×K	1054.64	Joback Method
cpg	1545.91	J/mol×K	1092.79	Joback Method
cpg	1564.79	J/mol×K	1130.94	Joback Method
cpg	1582.75	J/mol×K	1169.09	Joback Method
cpg	1599.94	J/mol×K	1207.23	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=U415857&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