Benzamide, 6-trifluoromethyl-2-fluoro-N-octadecyl-

Inchi: InChI=1S/C26H41F4NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-31-25(32)24-22

InchiKey: XKHHLMBXWCTGKQ-UHFFFAOYSA-N

Formula: C26H41F4NO

SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 459.60

Physical Properties

Property code	Value	Unit	Source
gf	-554.74	kJ/mol	Joback Method
hf	-1218.68	kJ/mol	Joback Method
hfus	67.96	kJ/mol	Joback Method
hvap	85.69	kJ/mol	Joback Method
log10ws	-10.37		Crippen Method
logp	8.836		Crippen Method
mcvol	372.070	ml/mol	McGowan Method
pc	817.26	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
tb	928.81	K	Joback Method
tc	1139.25	K	Joback Method
tf	541.61	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.04	J/mol×K	928.81	Joback Method
cpg	1273.23	J/mol×K	963.88	Joback Method
cpg	1291.23	J/mol×K	998.96	Joback Method
cpg	1308.12	J/mol×K	1034.03	Joback Method
cpg	1324.02	J/mol×K	1069.10	Joback Method
cpg	1339.00	J/mol×K	1104.17	Joback Method
cpg	1353.17	J/mol×K	1139.25	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=U406016&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