Benzamide, 2,4,5-trifluoro-3-methoxy-N-octadecyl-

Inchi: InChI=1S/C26H42F3NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-30-26(31)21-
InchiKey: KCOIZMLQGOKABR-UHFFFAOYSA-N
Formula: C26H42F3NO2
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 457.61

Physical Properties

Property code	Value	Unit	Source
gf	-487.03	kJ/mol	Joback Method
hf	-1168.98	kJ/mol	Joback Method
hfus	72.71	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	8.104		Crippen Method
mcvol	376.170	ml/mol	McGowan Method
pc	807.54	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
tb	965.15	K	Joback Method
tc	1187.63	K	Joback Method
tf	585.87	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.64	J/mol×K	965.15	Joback Method
cpg	1296.73	J/mol×K	1002.23	Joback Method
cpg	1314.29	J/mol×K	1039.31	Joback Method
cpg	1330.38	J/mol×K	1076.39	Joback Method
cpg	1345.04	J/mol×K	1113.47	Joback Method
cpg	1358.35	J/mol×K	1150.55	Joback Method
cpg	1370.35	J/mol×K	1187.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407652&Units=SI
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

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

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