2,4,5-Trifluoro-3-methoxybenzamide, N-(2-octyl)-

Inchi: InChI=1S/C16H22F3NO2/c1-4-5-6-7-8-10(2)20-16(21)11-9-12(17)14(19)15(22-3)13(11)1

InchiKey: ACWHZKJYXTYDLE-UHFFFAOYSA-N

Formula: C16H22F3NO2

SMILES: CCCCCCC(C)NC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 317.35

Physical Properties

Property code	Value	Unit	Source
gf	-573.67	kJ/mol	Joback Method
hf	-967.86	kJ/mol	Joback Method
hfus	43.28	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.201		Crippen Method
mcvol	235.270	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2023.00		NIST Webbook
tb	735.91	K	Joback Method
tc	920.60	K	Joback Method
tf	458.17	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.95	J/mol×K	735.91	Joback Method
cpg	694.59	J/mol×K	766.69	Joback Method
cpg	708.43	J/mol×K	797.47	Joback Method
cpg	721.47	J/mol×K	828.25	Joback Method
cpg	733.73	J/mol×K	859.04	Joback Method
cpg	745.23	J/mol×K	889.82	Joback Method
cpg	755.97	J/mol×K	920.60	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=U358064&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