2-Fluoro-6-trifluoromethylbenzamide, N-(2-octyl)-

Inchi: InChI=1S/C16H21F4NO/c1-3-4-5-6-8-11(2)21-15(22)14-12(16(18,19)20)9-7-10-13(14)17

InchiKey: IOZMDSOFXKMOGD-UHFFFAOYSA-N

Formula: C16H21F4NO

SMILES: CCCCCCC(C)NC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 319.34

Physical Properties

Property code	Value	Unit	Source
gf	-641.38	kJ/mol	Joback Method
hf	-1017.56	kJ/mol	Joback Method
hfus	38.54	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.933		Crippen Method
mcvol	231.170	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	699.57	K	Joback Method
tc	883.23	K	Joback Method
tf	413.91	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.14	J/mol×K	699.57	Joback Method
cpg	678.04	J/mol×K	730.18	Joback Method
cpg	692.06	J/mol×K	760.79	Joback Method
cpg	705.25	J/mol×K	791.40	Joback Method
cpg	717.65	J/mol×K	822.01	Joback Method
cpg	729.30	J/mol×K	852.62	Joback Method
cpg	740.26	J/mol×K	883.23	Joback Method

Sources

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=U358112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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