4-(Methylthio)benzoic acid, 2,6-difluoro-«alpha»-methylbenzyl ester

Inchi: InChI=1S/C16H14F2O2S/c1-10(15-13(17)4-3-5-14(15)18)20-16(19)11-6-8-12(21-2)9-7-1

InchiKey: NJXVPUSXNDCSHK-UHFFFAOYSA-N

Formula: C16H14F2O2S

SMILES: CSc1ccc(C(=O)OC(C)c2c(F)cccc2F)cc1

Mol. weight [g/mol]: 308.34

Physical Properties

Property code	Value	Unit	Source
gf	-313.09	kJ/mol	Joback Method
hf	-535.35	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.605		Crippen Method
mcvol	216.110	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2272.00		NIST Webbook
tb	776.95	K	Joback Method
tc	1011.18	K	Joback Method
tf	453.22	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.33	J/mol×K	776.95	Joback Method
cpg	598.93	J/mol×K	815.99	Joback Method
cpg	611.33	J/mol×K	855.03	Joback Method
cpg	622.56	J/mol×K	894.06	Joback Method
cpg	632.66	J/mol×K	933.10	Joback Method
cpg	641.65	J/mol×K	972.14	Joback Method
cpg	649.55	J/mol×K	1011.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375070&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

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