

3-Methoxybenzoic acid, 2-fluoro-6-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C16H12F4O3/c1-22-11-5-2-4-10(8-11)15(21)23-9-12-13(16(18,19)20)6-3-7-14
InchiKey: IPZKKZJBHMQWLS-UHFFFAOYSA-N
Formula: C16H12F4O3
SMILES: COc1cccc(C(=O)OCc2c(F)cccc2C(F)(F)F)c1
Mol. weight [g/mol]: 328.26

Physical Properties

Property code	Value	Unit	Source
gf	-835.55	kJ/mol	Joback Method
hf	-1105.13	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.210		Crippen Method
mcvol	209.170	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	726.34	K	Joback Method
tc	934.03	K	Joback Method
tf	459.65	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.28	J/molxK	726.34	Joback Method
cpg	589.29	J/molxK	760.95	Joback Method
cpg	601.33	J/molxK	795.57	Joback Method
cpg	612.43	J/molxK	830.18	Joback Method
cpg	622.62	J/molxK	864.80	Joback Method
cpg	631.94	J/molxK	899.41	Joback Method
cpg	640.43	J/molxK	934.03	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=U374932&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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