6-Fluoro-2-trifluoromethylbenzoic acid, pentafluorobenzyl ester

Other names: 6-Fluoro-2-trifluorobenzoic acid, pentafluorobenzyl ester
Inchi: InChI=1S/C15H5F9O2/c16-7-3-1-2-6(15(22,23)24)8(7)14(25)26-4-5-9(17)11(19)13(21)12
InchiKey: LNTSJUQBLQNSHP-UHFFFAOYSA-N
Formula: C15H5F9O2
SMILES: O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 388.18

Physical Properties

Property code	Value	Unit	Source
gf	-1751.54	kJ/mol	Joback Method
hf	-1978.70	kJ/mol	Joback Method
hfus	43.06	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	4.897		Crippen Method
mcvol	198.060	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	697.31	K	Joback Method
tc	877.52	K	Joback Method
tf	479.18	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.92	J/mol×K	697.31	Joback Method
cpg	543.89	J/mol×K	727.35	Joback Method
cpg	553.23	J/mol×K	757.38	Joback Method
cpg	561.95	J/mol×K	787.42	Joback Method
cpg	570.07	J/mol×K	817.45	Joback Method
cpg	577.61	J/mol×K	847.49	Joback Method
cpg	584.58	J/mol×K	877.52	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=U343738&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