

6-Fluoro-3-trifluoromethylbenzoic acid, pentafluorobenzyl ester

Other names:	6-Fluoro-3-trifluorobenzoic acid, pentafluorobenzyl ester
Inchi:	InChI=1S/C15H5F9O2/c16-8-2-1-5(15(22,23)24)3-6(8)14(25)26-4-7-9(17)11(19)13(21)12
InchiKey:	UBBCOIQITAJGCO-UHFFFAOYSA-N
Formula:	C15H5F9O2
SMILES:	O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1cc(C(F)(F)F)ccc1F
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	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	697.31	K	Joback Method
tc	877.52	K	Joback Method
tf	479.18	K	Joback Method
vc	0.835	m ³ /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

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=U343784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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