

Isophthalic acid, pentafluorobenzyl pentyl ester

Inchi:	InChI=1S/C20H17F5O4/c1-2-3-4-8-28-19(26)11-6-5-7-12(9-11)20(27)29-10-13-14(21)16
InchiKey:	GDZWBFXTGVPMMF-UHFFFAOYSA-N
Formula:	C20H17F5O4
SMILES:	CCCCCOC(=O)c1ccccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]:	416.34

Physical Properties

Property code	Value	Unit	Source
gf	-1157.33	kJ/mol	Joback Method
hf	-1522.04	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.086		Crippen Method
mcvol	268.870	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook
tb	889.17	K	Joback Method
tc	1093.67	K	Joback Method
tf	590.39	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.97	J/mol×K	889.17	Joback Method
cpg	823.73	J/mol×K	923.25	Joback Method
cpg	834.40	J/mol×K	957.34	Joback Method
cpg	844.00	J/mol×K	991.42	Joback Method
cpg	852.52	J/mol×K	1025.51	Joback Method
cpg	859.98	J/mol×K	1059.59	Joback Method
cpg	866.38	J/mol×K	1093.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344504&Units=SI

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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