

Isophthalic acid, nonyl pentafluorobenzyl ester

Inchi:	InChI=1S/C24H25F5O4/c1-2-3-4-5-6-7-8-12-32-23(30)15-10-9-11-16(13-15)24(31)33-14
InchiKey:	AZKZTGAXNUTUPS-UHFFFAOYSA-N
Formula:	C24H25F5O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]:	472.44

Physical Properties

Property code	Value	Unit	Source
gf	-1123.65	kJ/mol	Joback Method
hf	-1604.60	kJ/mol	Joback Method
hfus	64.64	kJ/mol	Joback Method
hvap	91.77	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	6.647		Crippen Method
mcvol	325.230	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	980.69	K	Joback Method
tc	1200.93	K	Joback Method
tf	635.47	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.74	J/molxK	980.69	Joback Method
cpg	1058.46	J/molxK	1017.40	Joback Method
cpg	1069.74	J/molxK	1054.10	Joback Method
cpg	1079.62	J/molxK	1090.81	Joback Method
cpg	1088.11	J/molxK	1127.52	Joback Method
cpg	1095.23	J/molxK	1164.22	Joback Method
cpg	1101.02	J/molxK	1200.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U344508&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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