

Isophthalic acid, hexyl 2-nitro-5-fluorophenyl ester

Inchi:	InChI=1S/C20H20FNO6/c1-2-3-4-5-11-27-19(23)14-7-6-8-15(12-14)20(24)28-18-13-16(2
InchiKey:	XBFLOHFDOFLPPK-UHFFFAOYSA-N
Formula:	C20H20FNO6
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1
Mol. weight [g/mol]:	389.37

Physical Properties

Property code	Value	Unit	Source
gf	-313.65	kJ/mol	Joback Method
hf	-713.95	kJ/mol	Joback Method
hfus	54.49	kJ/mol	Joback Method
hvap	100.74	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	4.690		Crippen Method
mvol	279.210	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	1028.99	K	Joback Method
tc	1269.87	K	Joback Method
tf	694.08	K	Joback Method
vc	1.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.96	J/molxK	1028.99	Joback Method
cpg	890.31	J/molxK	1069.14	Joback Method
cpg	898.24	J/molxK	1109.28	Joback Method
cpg	904.80	J/molxK	1149.43	Joback Method
cpg	910.04	J/molxK	1189.58	Joback Method
cpg	913.97	J/molxK	1229.73	Joback Method
cpg	916.66	J/molxK	1269.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U344421&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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