

Anthralin, O,O',O''-tri(pentafluoropropionyl)-

Inchi:	InChI=1S/C23H7F15O6/c24-18(25,21(30,31)32)15(39)42-10-5-1-3-8-7-9-4-2-6-11(43-16)
InchiKey:	NCPYBGRXPRVWEE-UHFFFAOYSA-N
Formula:	C23H7F15O6
SMILES:	O=C(Oc1cccc2cc3cccc(OC(=O)C(F)(F)C(F)(F)F)c3c(OC(=O)C(F)(F)C(F)(F)F)c12)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	664.27

Physical Properties

Property code	Value	Unit	Source
gf	-3176.90	kJ/mol	Joback Method
hf	-3673.81	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	7.302		Crippen Method
mvol	321.120	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	1008.74	K	Joback Method
tc	1238.20	K	Joback Method
tf	730.72	K	Joback Method
vc	1.335	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.20	J/molxK	1008.74	Joback Method
cpg	1042.29	J/molxK	1046.98	Joback Method
cpg	1051.29	J/molxK	1085.23	Joback Method
cpg	1060.41	J/molxK	1123.47	Joback Method
cpg	1069.88	J/molxK	1161.71	Joback Method
cpg	1079.94	J/molxK	1199.96	Joback Method
cpg	1090.81	J/molxK	1238.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374299&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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