

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

Inchi:	InChI=1S/C20H7F9O6/c21-18(22,23)15(30)33-10-5-1-3-8-7-9-4-2-6-11(34-16(31)19(24,25)12)3
InchiKey:	CEUXARQAGXSIAX-UHFFFAOYSA-N
Formula:	C20H7F9O6
SMILES:	O=C(Oc1cccc2cc3cccc(OC(=O)C(F)(F)F)c3c(OC(=O)C(F)(F)F)c12)C(F)(F)F
Mol. weight [g/mol]:	514.25

Physical Properties

Property code	Value	Unit	Source
gf	-2041.82	kJ/mol	Joback Method
hf	-2408.98	kJ/mol	Joback Method
hfus	47.92	kJ/mol	Joback Method
hvap	84.54	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	5.396		Crippen Method
mcvol	268.230	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinqol	2150.00		NIST Webbook
tb	954.17	K	Joback Method
tc	1170.53	K	Joback Method
tf	686.11	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.45	J/molxK	954.17	Joback Method
cpg	827.43	J/molxK	990.23	Joback Method
cpg	834.84	J/molxK	1026.29	Joback Method
cpg	841.80	J/molxK	1062.35	Joback Method
cpg	848.41	J/molxK	1098.41	Joback Method
cpg	854.78	J/molxK	1134.47	Joback Method
cpg	861.03	J/molxK	1170.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374846&Units=SI
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

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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