

C9H2F18O4S2

Inchi:	InChI=1S/C9H2F18O4S2/c10-2(11,6(18,19)20)4(14,15)8(24,25)32(28,29)1-33(30,31)9(2
InchiKey:	XONFSEOHZGSMJG-UHFFFAOYSA-N
Formula:	C9H2F18O4S2
SMILES:	O=S(=O)(CS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	580.21
CAS:	29214-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-4396.04	kJ/mol	Joback Method
hf	-4735.77	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.625		Crippen Method
mcvol	225.710	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
tb	461.90	K	Joback Method
tc	577.29	K	Joback Method
tf	298.29	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.73	J/molxK	461.90	Joback Method
cpg	614.91	J/molxK	481.13	Joback Method
cpg	627.30	J/molxK	500.36	Joback Method
cpg	638.92	J/molxK	519.60	Joback Method
cpg	649.80	J/molxK	538.83	Joback Method
cpg	659.97	J/molxK	558.06	Joback Method
cpg	669.46	J/molxK	577.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29214377&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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