

Acetic acid, [(7-oxo-7h-benz[de]anthracen-3-yl)thio]-

Inchi:	InChI=1S/C19H12O3S/c20-17(21)10-23-16-9-8-12-11-4-1-2-5-13(11)19(22)15-7-3-6-14(
InchiKey:	QQRGUQLAJOQLIW-UHFFFAOYSA-N
Formula:	C19H12O3S
SMILES:	O=C(O)CSc1ccc2c3c(cccc13)C(=O)c1ccccc1-2
Mol. weight [g/mol]:	320.36
CAS:	69658-13-5

Physical Properties

Property code	Value	Unit	Source
gf	139.50	kJ/mol	Joback Method
hf	-72.42	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	101.09	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.228		Crippen Method
mvol	226.090	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	1011.90	K	Joback Method
tc	1268.12	K	Joback Method
tf	682.10	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.44	J/molxK	1011.90	Joback Method
cpg	675.70	J/molxK	1054.60	Joback Method
cpg	685.58	J/molxK	1097.31	Joback Method
cpg	695.22	J/molxK	1140.01	Joback Method
cpg	704.75	J/molxK	1182.71	Joback Method
cpg	714.33	J/molxK	1225.41	Joback Method
cpg	724.07	J/molxK	1268.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69658135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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