

(Phenylthio)acetic acid, 1-adamantylmethyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H24O2S/c20-18(12-22-17-4-2-1-3-5-17)21-13-19-9-14-6-15(10-19)8-16(7-

OBBPJCYJLUECGQ-UHFFFAOYSA-N

C19H24O2S

O=C(CSc1ccccc1)OCC12CC3CC(CC(C3)C1)C2

316.46

Physical Properties

Property code	Value	Unit	Source
gf	177.66	kJ/mol	Joback Method
hf	-194.75	kJ/mol	Joback Method
hfus	33.00	kJ/mol	Joback Method
hvap	74.59	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.538		Crippen Method
mcvol	246.020	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	825.93	K	Joback Method
tc	1076.04	K	Joback Method
tf	506.83	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.45	J/molxK	825.93	Joback Method
cpg	807.11	J/molxK	867.61	Joback Method
cpg	827.16	J/molxK	909.30	Joback Method
cpg	846.90	J/molxK	950.98	Joback Method
cpg	866.63	J/molxK	992.67	Joback Method
cpg	886.65	J/molxK	1034.35	Joback Method
cpg	907.25	J/molxK	1076.04	Joback Method

Sources

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=U299957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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