

(Phenylthio)acetic acid, undec-2-enyl ester

Inchi: InChI=1S/C19H28O2S/c1-2-3-4-5-6-7-8-9-13-16-21-19(20)17-22-18-14-11-10-12-15-18/
InchiKey: VGHZOGOKLCZGIS-UKTHLTGXSA-N
Formula: C19H28O2S
SMILES: CCCCCCCC=CCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 320.49

Physical Properties

Property code	Value	Unit	Source
gf	100.93	kJ/mol	Joback Method
hf	-284.67	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.629		Crippen Method
mvol	274.300	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	810.03	K	Joback Method
tc	1019.99	K	Joback Method
tf	431.79	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.87	J/molxK	810.03	Joback Method
cpg	823.53	J/molxK	845.02	Joback Method
cpg	839.07	J/molxK	880.02	Joback Method
cpg	853.55	J/molxK	915.01	Joback Method
cpg	867.00	J/molxK	950.00	Joback Method
cpg	879.49	J/molxK	985.00	Joback Method
cpg	891.06	J/molxK	1019.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299427&Units=SI

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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