

(Phenylthio)acetic acid, tridec-2-ynyl ester

Inchi:	InChI=1S/C21H30O2S/c1-2-3-4-5-6-7-8-9-10-11-15-18-23-21(22)19-24-20-16-13-12-14-
InchiKey:	SULJTZRRVIWJGU-UHFFFAOYSA-N
Formula:	C21H30O2S
SMILES:	CCCCCCCCCCC#CCOC(=O)CSc1ccccc1
Mol. weight [g/mol]:	346.53

Physical Properties

Property code	Value	Unit	Source
gf	240.35	kJ/mol	Joback Method
hf	-170.87	kJ/mol	Joback Method
hfus	54.23	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.856		Crippen Method
mcvol	298.180	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2845.00		NIST Webbook
tb	860.63	K	Joback Method
tc	1077.52	K	Joback Method
tf	565.51	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.19	J/molxK	860.63	Joback Method
cpg	915.99	J/molxK	896.78	Joback Method
cpg	931.53	J/molxK	932.93	Joback Method
cpg	945.87	J/molxK	969.07	Joback Method
cpg	959.03	J/molxK	1005.22	Joback Method
cpg	971.08	J/molxK	1041.37	Joback Method
cpg	982.04	J/molxK	1077.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299428&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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