

Ethyl (phenylthio)acetate

Other names:	Ethyl (phenylsulfanyl)acetate (Phenylthio)acetic acid, ethyl ester Acetic acid, (phenylthio)-, ethyl ester
Inchi:	InChI=1S/C10H12O2S/c1-2-12-10(11)8-13-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	SEDRTXNDGKRHBL-UHFFFAOYSA-N
Formula:	C10H12O2S
SMILES:	CCOC(=O)CSc1ccccc1
Mol. weight [g/mol]:	196.27
CAS:	7605-25-6

Physical Properties

Property code	Value	Unit	Source
gf	-55.07	kJ/mol	Joback Method
hf	-216.13	kJ/mol	Joback Method
hfus	22.61	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.342		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	599.95	K	Joback Method
tc	831.45	K	Joback Method
tf	335.44	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.90	J/mol×K	599.95	Joback Method
cpg	364.55	J/mol×K	638.53	Joback Method
cpg	377.31	J/mol×K	677.12	Joback Method

cpg	389.18	J/mol×K	715.70	Joback Method
cpg	400.18	J/mol×K	754.28	Joback Method
cpg	410.33	J/mol×K	792.87	Joback Method
cpg	419.64	J/mol×K	831.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7605256&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
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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