(Phenylthio)acetic acid, tridecyl ester

Inchi: InChI=1S/C21H34O2S/c1-2-3-4-5-6-7-8-9-10-11-15-18-23-21(22)19-24-20-16-13-12-14-1
InchiKey: AZPHKVXGGROXDY-UHFFFAOYSA-N
Formula: C21H34O2S
SMILES: CCCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 350.56

Physical Properties

Property code	Value	Unit	Source
gf	37.55	kJ/mol	Joback Method
hf	-443.17	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	80.59	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.633		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2612.00		NIST Webbook
tb	851.63	K	Joback Method
tc	1055.74	K	Joback Method
tf	459.41	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.98	J/mol×K	851.63	Joback Method
cpg	968.39	J/mol×K	885.65	Joback Method
cpg	984.60	J/mol×K	919.67	Joback Method
cpg	999.64	J/mol×K	953.69	Joback Method
cpg	1013.56	J/mol×K	987.70	Joback Method
cpg	1026.40	J/mol×K	1021.72	Joback Method
cpg	1038.19	J/mol×K	1055.74	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=U299850&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume