(Phenylthio)acetic acid, dodecyl ester

Inchi: InChI=1S/C20H32O2S/c1-2-3-4-5-6-7-8-9-10-14-17-22-20(21)18-23-19-15-12-11-13-16-1
InchiKey: UZXYYFYUFDWZCI-UHFFFAOYSA-N
Formula: C20H32O2S
SMILES: CCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 336.53

Physical Properties

Property code	Value	Unit	Source
gf	29.13	kJ/mol	Joback Method
hf	-422.53	kJ/mol	Joback Method
hfus	48.51	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.243		Crippen Method
mcvol	292.690	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2508.00		NIST Webbook
rinpol	2508.00		NIST Webbook
tb	828.75	K	Joback Method
tc	1032.71	K	Joback Method
tf	448.14	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.34	J/mol×K	828.75	Joback Method
cpg	908.60	J/mol×K	862.74	Joback Method
cpg	924.69	J/mol×K	896.74	Joback Method
cpg	939.64	J/mol×K	930.73	Joback Method
cpg	953.48	J/mol×K	964.72	Joback Method
cpg	966.27	J/mol×K	998.71	Joback Method
cpg	978.03	J/mol×K	1032.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299849&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume