

Cysteine, s-(diphenylmethyl)-l-

Inchi:	InChI=1S/C16H17NO2S/c17-14(16(18)19)11-20-15(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1
InchiKey:	SHOGZCIBPYFZRP-UHFFFAOYSA-N
Formula:	C16H17NO2S
SMILES:	NC(CSC(c1ccccc1)c1ccccc1)C(=O)O
Mol. weight [g/mol]:	287.38
CAS:	39825-30-4

Physical Properties

Property code	Value	Unit	Source
gf	137.61	kJ/mol	Joback Method
hf	-100.22	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.921		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
tb	905.32	K	Joback Method
tc	1149.97	K	Joback Method
tf	521.33	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.49	J/molxK	905.32	Joback Method
cpg	666.35	J/molxK	946.09	Joback Method
cpg	676.13	J/molxK	986.87	Joback Method
cpg	684.91	J/molxK	1027.64	Joback Method
cpg	692.79	J/molxK	1068.42	Joback Method
cpg	699.85	J/molxK	1109.19	Joback Method
cpg	706.18	J/molxK	1149.97	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=C39825304&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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