l-Cysteine, N,S-bis(caproyl)-, methyl ester

Inchi: InChI=1S/C16H29NO4S/c1-4-6-8-10-14(18)17-13(16(20)21-3)12-22-15(19)11-9-7-5-2/h1
InchiKey: YCIZSACBLKKKCO-UHFFFAOYSA-N
Formula: C16H29NO4S
SMILES: CCCCCC(=O)NC(CSC(=O)CCCCC)C(=O)OC
Mol. weight [g/mol]: 331.47

Physical Properties

Property code	Value	Unit	Source
gf	-287.85	kJ/mol	Joback Method
hf	-753.47	kJ/mol	Joback Method
hfus	48.89	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.065		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2269.00		NIST Webbook
tb	868.02	K	Joback Method
tc	1071.41	K	Joback Method
tf	514.16	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.39	J/mol×K	868.02	Joback Method
cpg	859.53	J/mol×K	901.92	Joback Method
cpg	872.58	J/mol×K	935.82	Joback Method
cpg	884.55	J/mol×K	969.72	Joback Method
cpg	895.47	J/mol×K	1003.62	Joback Method
cpg	905.36	J/mol×K	1037.51	Joback Method
cpg	914.22	J/mol×K	1071.41	Joback Method

Sources

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=U299739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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