3-(2-Naphthylthio)propionic acid

Inchi: InChI=1S/C13H12O2S/c14-13(15)7-8-16-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,7-8H2,(H
InchiKey: XMQJAJQNGNSZFY-UHFFFAOYSA-N
Formula: C13H12O2S
SMILES: O=C(O)CCSc1ccc2ccccc2c1
Mol. weight [g/mol]: 232.30
CAS: 1141-45-3

Physical Properties

Property code	Value	Unit	Source
gf	35.39	kJ/mol	Joback Method
hf	-118.46	kJ/mol	Joback Method
hfus	29.91	kJ/mol	Joback Method
hvap	79.35	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.407		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	762.31	K	Joback Method
tc	992.29	K	Joback Method
tf	453.06	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.27	J/mol×K	762.31	Joback Method
cpg	467.98	J/mol×K	800.64	Joback Method
cpg	477.86	J/mol×K	838.97	Joback Method
cpg	487.00	J/mol×K	877.30	Joback Method
cpg	495.44	J/mol×K	915.63	Joback Method
cpg	503.27	J/mol×K	953.96	Joback Method
cpg	510.54	J/mol×K	992.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1141453&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume