

3,3'-Dithiobis[2-amino-n-(2-naphthyl)propionamid

Inchi:	InChI=1S/C26H26N4O2S2/c27-23(25(31)29-21-11-9-17-5-1-3-7-19(17)13-21)15-33-34-1
InchiKey:	REEVAJUPLLLWYBH-UHFFFAOYSA-N
Formula:	C26H26N4O2S2
SMILES:	NC(CSSCC(N)C(=O)Nc1ccc2ccccc2c1)C(=O)Nc1ccc2ccccc2c1
Mol. weight [g/mol]:	490.64
CAS:	4708-24-1

Physical Properties

Property code	Value	Unit	Source
gf	702.10	kJ/mol	Joback Method
hf	274.83	kJ/mol	Joback Method
hfus	69.44	kJ/mol	Joback Method
hvap	143.13	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	4.606		Crippen Method
mvol	366.520	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
tb	1385.38	K	Joback Method
tc	1696.13	K	Joback Method
tf	936.56	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.23	J/molxK	1385.38	Joback Method
cpg	1240.86	J/molxK	1437.17	Joback Method
cpg	1256.51	J/molxK	1488.96	Joback Method
cpg	1273.54	J/molxK	1540.75	Joback Method
cpg	1292.31	J/molxK	1592.54	Joback Method
cpg	1313.17	J/molxK	1644.33	Joback Method
cpg	1336.49	J/molxK	1696.13	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=C4708241&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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