

N,n'-[2,2'-dithiobis(ethyloctanamide)]

Inchi:	InChI=1S/C20H40N2O2S2/c1-3-5-7-9-11-13-19(23)21-15-17-25-26-18-16-22-20(24)14-1
InchiKey:	ZSJMBESDVGXBCP-UHFFFAOYSA-N
Formula:	C20H40N2O2S2
SMILES:	CCCCCCCC(=O)NCCSSCCNC(=O)CCCCCCC
Mol. weight [g/mol]:	404.67
CAS:	96123-64-7

Physical Properties

Property code	Value	Unit	Source
gf	104.70	kJ/mol	Joback Method
hf	-490.61	kJ/mol	Joback Method
hfus	69.21	kJ/mol	Joback Method
hvap	100.11	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.321		Crippen Method
mcvol	348.460	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
tb	1002.64	K	Joback Method
tc	1227.58	K	Joback Method
tf	589.14	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.27	J/molxK	1002.64	Joback Method
cpg	1172.39	J/molxK	1040.13	Joback Method
cpg	1186.11	J/molxK	1077.62	Joback Method
cpg	1198.49	J/molxK	1115.11	Joback Method
cpg	1209.57	J/molxK	1152.60	Joback Method
cpg	1219.41	J/molxK	1190.09	Joback Method
cpg	1228.08	J/molxK	1227.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C96123647&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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