N,N-Diethylthiobenzamide

Inchi: InChI=1S/C11H15NS/c1-3-12(4-2)11(13)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey: BLKHEHXBEXPSAR-UHFFFAOYSA-N
Formula: C11H15NS
SMILES: CCN(CC)C(=S)c1ccccc1
Mol. weight [g/mol]: 193.31
CAS: 18775-06-9

Physical Properties

Property code	Value	Unit	Source
chs	-7064.00 ± 1.50	kJ/mol	NIST Webbook
gf	381.99	kJ/mol	Joback Method
hf	81.10 ± 3.80	kJ/mol	NIST Webbook
hfs	-10.30 ± 2.10	kJ/mol	NIST Webbook
hfus	25.91	kJ/mol	Joback Method
hsub	91.40 ± 3.20	kJ/mol	NIST Webbook
hvap	51.13	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.704		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	560.24	K	Joback Method
tc	784.70	K	Joback Method
tf	306.89	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.68	J/mol×K	560.24	Joback Method
cpg	388.22	J/mol×K	597.65	Joback Method
cpg	402.61	J/mol×K	635.06	Joback Method
cpg	415.94	J/mol×K	672.47	Joback Method
cpg	428.30	J/mol×K	709.88	Joback Method
cpg	439.78	J/mol×K	747.29	Joback Method

cpg	450.47	J/mol×K	784.70	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=C18775069&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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