2-Phenylnaphthylsulfide

Inchi: InChI=1S/C16H12S/c1-2-8-15(9-3-1)17-16-11-10-13-6-4-5-7-14(13)12-16/h1-12H
InchiKey: APWYHOPXAIRDIZ-UHFFFAOYSA-N
Formula: C16H12S
SMILES: c1ccc(Sc2ccc3ccccc3c2)cc1
Mol. weight [g/mol]: 236.33
CAS: 7570-96-9

Physical Properties

Property code	Value	Unit	Source
gf	438.80	kJ/mol	Joback Method
hf	320.96	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.991		Crippen Method
mcvol	185.670	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	364.94		NIST Webbook
rinpol	364.94		NIST Webbook
tb	711.58	K	Joback Method
tc	991.64	K	Joback Method
tf	402.54	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.10	J/mol×K	711.58	Joback Method
cpg	479.84	J/mol×K	758.26	Joback Method
cpg	494.06	J/mol×K	804.93	Joback Method
cpg	506.91	J/mol×K	851.61	Joback Method
cpg	518.55	J/mol×K	898.28	Joback Method
cpg	529.14	J/mol×K	944.96	Joback Method
cpg	538.84	J/mol×K	991.64	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=C7570969&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

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