2-Phenylbenzo-1,4-thiazane-3-one

Inchi: InChI=1S/C14H11NOS/c16-14-13(10-6-2-1-3-7-10)17-12-9-5-4-8-11(12)15-14/h1-9,13H,
InchiKey: DLALSZUJBMNOHZ-UHFFFAOYSA-N
Formula: C14H11NOS
SMILES: O=C1Nc2ccccc2SC1c1ccccc1
Mol. weight [g/mol]: 241.31
CAS: 38533-19-6

Physical Properties

Property code	Value	Unit	Source
gf	335.82	kJ/mol	Joback Method
hf	141.31	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.472		Crippen Method
mcvol	177.640	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	753.27	K	Joback Method
tc	1045.45	K	Joback Method
tf	584.02	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.15	J/mol×K	753.27	Joback Method
cpg	490.27	J/mol×K	801.97	Joback Method
cpg	504.75	J/mol×K	850.66	Joback Method
cpg	517.66	J/mol×K	899.36	Joback Method
cpg	529.08	J/mol×K	948.06	Joback Method
cpg	539.09	J/mol×K	996.76	Joback Method
cpg	547.77	J/mol×K	1045.45	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=C38533196&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume