DL-Goitrin

Inchi: InChI=1S/C5H7NOS/c1-2-4-3-6-5(8)7-4/h2,4H,1,3H2,(H,6,8)
InchiKey: UZQVYLOFLQICCT-UHFFFAOYSA-N
Formula: C5H7NOS
SMILES: C=CC1CNC(=S)O1
Mol. weight [g/mol]: 129.18

Physical Properties

Property code	Value	Unit	Source
hfus	24.96	kJ/mol	Joback Method
logp	0.446		Crippen Method
mcvol	94.050	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.42	J/mol×K	473.90	Joback Method
cpg	192.71	J/mol×K	513.34	Joback Method
cpg	202.27	J/mol×K	552.78	Joback Method
cpg	211.17	J/mol×K	592.22	Joback Method
cpg	219.43	J/mol×K	631.66	Joback Method
cpg	227.12	J/mol×K	671.10	Joback Method
cpg	234.27	J/mol×K	710.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C13190346

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume