P-propionotoluidide, 3-mercapto-

Inchi: InChI=1S/C10H13NOS/c1-8-2-4-9(5-3-8)11-10(12)6-7-13/h2-5,13H,6-7H2,1H3,(H,11,12)
InchiKey: GFSJBUDXTRNXAV-UHFFFAOYSA-N
Formula: C10H13NOS
SMILES: Cc1ccc(NC(=O)CCS)cc1
Mol. weight [g/mol]: 195.28
CAS: 78580-32-2

Physical Properties

Property code	Value	Unit	Source
gf	125.96	kJ/mol	Joback Method
hf	-45.30	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	60.71	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.253		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	626.76	K	Joback Method
tc	861.35	K	Joback Method
tf	380.45	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.24	J/mol×K	626.76	Joback Method
cpg	384.61	J/mol×K	665.86	Joback Method
cpg	397.04	J/mol×K	704.96	Joback Method
cpg	408.58	J/mol×K	744.06	Joback Method
cpg	419.27	J/mol×K	783.16	Joback Method
cpg	429.15	J/mol×K	822.26	Joback Method
cpg	438.25	J/mol×K	861.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78580322&Units=SI
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

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

Latest version available from:
https://www.chemeo.com/cid/94-405-8/P-propionotoluidide-3-mercapto.pdf
Generated by Cheméo on 2024-04-20 05:58:43.969196587 +0000 UTC m=+15881972.889773903.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.