Dipropenyl disulfide

Inchi: InChI=1S/C6H10S2/c1-3-5-7-8-6-4-2/h3-6H,1-2H3/b5-3-,6-4-
InchiKey: FHSDVOJKLYJNCQ-GLIMQPGKSA-N
Formula: C6H10S2
SMILES: CC=CSSC=CC
Mol. weight [g/mol]: 146.27
CAS: 23838-22-4

Physical Properties

Property code	Value	Unit	Source
gf	226.32	kJ/mol	Joback Method
hf	151.01	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	42.50	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.435		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1099.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1120.20		NIST Webbook
tb	482.56	K	Joback Method
tc	716.77	K	Joback Method
tf	216.02	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.51	J/mol×K	482.56	Joback Method
cpg	230.71	J/mol×K	521.60	Joback Method
cpg	241.19	J/mol×K	560.63	Joback Method
cpg	250.99	J/mol×K	599.67	Joback Method

cpg	260.15	J/mol×K	638.70	Joback Method
cpg	268.71	J/mol×K	677.74	Joback Method
cpg	276.70	J/mol×K	716.77	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=C23838224&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume