E-(3-Chloro-2-methyl-allylsulfanyl)methyl-benzene

Other names: E-(3-Chloro-2-methyl-allylthio)-methyl benzene
Inchi: InChI=1S/C11H13ClS/c1-10(7-12)8-13-9-11-5-3-2-4-6-11/h2-7H,8-9H2,1H3/b10-7+
InchiKey: MTEZNPWGPCHQBQ-JXMROGBWSA-N
Formula: C11H13ClS
SMILES: CC(=CCl)CSCc1ccccc1
Mol. weight [g/mol]: 212.74

Physical Properties

Property code	Value	Unit	Source
gf	247.01	kJ/mol	Joback Method
hf	99.72	kJ/mol	Joback Method
hfus	25.51	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.062		Crippen Method
mcvol	166.380	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1619.70		NIST Webbook
ripol	2616.20		NIST Webbook
tb	588.01	K	Joback Method
tc	829.32	K	Joback Method
tf	285.43	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.68	J/mol×K	588.01	Joback Method
cpg	378.51	J/mol×K	628.23	Joback Method
cpg	392.24	J/mol×K	668.45	Joback Method
cpg	404.93	J/mol×K	708.67	Joback Method
cpg	416.66	J/mol×K	748.88	Joback Method
cpg	427.49	J/mol×K	789.10	Joback Method
cpg	437.49	J/mol×K	829.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R388871&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume