«delta»-3-isopentenylmethyl sulfide

Inchi: InChI=1S/C6H12S/c1-6(2)4-5-7-3/h1,4-5H2,2-3H3
InchiKey: UTEDUYINKYCEKZ-UHFFFAOYSA-N
Formula: C6H12S
SMILES: C=C(C)CCSC
Mol. weight [g/mol]: 116.22
CAS: 5952-75-0

Physical Properties

Property code	Value	Unit	Source
gf	112.05	kJ/mol	Joback Method
hf	-9.66	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	35.18	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.316		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
ripol	1191.00		NIST Webbook
ripol	1191.00		NIST Webbook
tb	402.02	K	Joback Method
tc	598.97	K	Joback Method
tf	176.06	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.59	J/mol×K	402.02	Joback Method
cpg	202.58	J/mol×K	434.84	Joback Method
cpg	213.09	J/mol×K	467.67	Joback Method
cpg	223.14	J/mol×K	500.49	Joback Method
cpg	232.74	J/mol×K	533.32	Joback Method
cpg	241.89	J/mol×K	566.14	Joback Method
cpg	250.62	J/mol×K	598.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5952750&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume