(4S,7S)-7-isopropyl-4methyloxepane-2-thione

Inchi: InChI=1S/C10H18OS/c1-7(2)9-5-4-8(3)6-10(12)11-9/h7-9H,4-6H2,1-3H3/t8-,9+/m1/s1
InchiKey: HRMAROUHNNJJLG-BDAKNGLRSA-N
Formula: C10H18OS
SMILES: CC1CCC(C(C)C)OC(=S)C1
Mol. weight [g/mol]: 186.31

Physical Properties

Property code	Value	Unit	Source
gf	40.25	kJ/mol	Joback Method
hf	-244.09	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.175		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1462.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	546.50	K	Joback Method
tc	774.46	K	Joback Method
tf	277.32	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.06	J/mol×K	546.50	Joback Method
cpg	399.98	J/mol×K	584.49	Joback Method
cpg	417.76	J/mol×K	622.49	Joback Method
cpg	434.45	J/mol×K	660.48	Joback Method
cpg	450.07	J/mol×K	698.48	Joback Method
cpg	464.67	J/mol×K	736.47	Joback Method
cpg	478.27	J/mol×K	774.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422461&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