ALLYL THIOPROPIONATE

Inchi: InChI=1S/C6H10OS/c1-3-5-8-6(7)4-2/h3H,1,4-5H2,2H3
InchiKey: GKRISGLFPMFKSX-UHFFFAOYSA-N
Formula: C6H10OS
SMILES: C=CCSC(=O)CC
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
hf	-168.44	kJ/mol	Cheméo Relay (1.0)
hfus	15.74	kJ/mol	Joback Method
hvap	44.16	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
logp	1.842		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
rinpol	709.00		NIST Webbook
rinpol	709.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.07	J/mol×K	456.01	Joback Method
cpg	217.17	J/mol×K	490.20	Joback Method
cpg	226.79	J/mol×K	524.39	Joback Method
cpg	235.94	J/mol×K	558.58	Joback Method
cpg	244.62	J/mol×K	592.78	Joback Method
cpg	252.85	J/mol×K	626.97	Joback Method
cpg	260.64	J/mol×K	661.16	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41820228&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices