

Sulfide, allyl sec-butyl

Other names:	Sulfide, allyl sec-butyl,
Inchi:	InChI=1S/C7H14S/c1-4-6-8-7(3)5-2/h4,7H,1,5-6H2,2-3H3
InchiKey:	QLCUOCVKHIAUIL-UHFFFAOYSA-N
Formula:	C7H14S
SMILES:	C=CCSC(C)CC
Mol. weight [g/mol]:	130.26

Physical Properties

Property code	Value	Unit	Source
hf	-51.26	kJ/mol	Cheméo Relay (1.0)
hfus	13.21	kJ/mol	Joback Method
hvap	44.36	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
logp	2.704		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
tb	422.85	K	Cheméo Relay (1.0)
tf	158.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.95	J/mol×K	424.58	Joback Method
cpg	242.43	J/mol×K	457.22	Joback Method
cpg	254.37	J/mol×K	489.87	Joback Method
cpg	265.77	J/mol×K	522.51	Joback Method
cpg	276.65	J/mol×K	555.16	Joback Method
cpg	287.01	J/mol×K	587.80	Joback Method
cpg	296.87	J/mol×K	620.45	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C70289075&Units=SI>

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):

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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