2-(sulfanylmethyl)hexan-1-ol

Inchi: InChI=1S/C7H16OS/c1-3-4-5-7(6-8)9-2/h7-8H,3-6H2,1-2H3
InchiKey: XFZCXPPCDICCOC-UHFFFAOYSA-N
Formula: C7H16OS
SMILES: CCCCC(CO)SC
Mol. weight [g/mol]: 148.27

Physical Properties

Property code	Value	Unit	Source
hf	-313.62	kJ/mol	Cheméo Relay (1.0)
hfus	18.58	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-0.91		Cheméo Relay (1.0)
logp	1.901		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	1217.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	1985.00		NIST Webbook
tb	494.56	K	Cheméo Relay (1.0)
tc	687.01	K	Cheméo Relay (1.0)
tf	235.37	K	Cheméo Relay (1.0)
vc	0.446	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.21	J/mol×K	520.08	Joback Method
cpg	309.58	J/mol×K	550.46	Joback Method
cpg	320.47	J/mol×K	580.84	Joback Method
cpg	330.88	J/mol×K	611.22	Joback Method
cpg	340.83	J/mol×K	641.61	Joback Method
cpg	350.33	J/mol×K	671.99	Joback Method
cpg	359.37	J/mol×K	702.37	Joback Method

Sources

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=R419762&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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