4-Sulfanyl-4-methylpentan-1-ol

Inchi: InChI=1S/C6H14OS/c1-6(2,8)4-3-5-7/h7-8H,3-5H2,1-2H3
InchiKey: LYYCZSHAGOLATI-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CC(C)(S)CCCO
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
gf	-104.95	kJ/mol	Joback Method
hf	-289.67	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.467		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1838.00		NIST Webbook
tb	488.49	K	Joback Method
tc	679.97	K	Joback Method
tf	257.08	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.25	J/mol×K	488.49	Joback Method
cpg	267.15	J/mol×K	520.40	Joback Method
cpg	277.45	J/mol×K	552.32	Joback Method
cpg	287.17	J/mol×K	584.23	Joback Method
cpg	296.35	J/mol×K	616.14	Joback Method
cpg	305.01	J/mol×K	648.06	Joback Method

cpg	313.18	J/mol×K	679.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R621480&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

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