2-(Heptylsulfanyl)ethanol

Other names: Ethanol, 2-(heptylthio)-
Inchi: InChI=1S/C9H20OS/c1-2-3-4-5-6-8-11-9-7-10/h10H,2-9H2,1H3
InchiKey: SFQDKASLZODHCY-UHFFFAOYSA-N
Formula: C9H20OS
SMILES: CCCCCCCSCCO
Mol. weight [g/mol]: 176.33

Physical Properties

Property code	Value	Unit	Source
af	0.7417		Cheméo Relay (1.0)
gf	-78.80	kJ/mol	Joback Method
hf	-367.00	kJ/mol	Cheméo Relay (1.0)
hfus	27.28	kJ/mol	Joback Method
hvap	82.90	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-2.67		Cheméo Relay (1.0)
logp	2.682		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	537.89	K	Cheméo Relay (1.0)
tc	740.96	K	Cheméo Relay (1.0)
tf	263.60	K	Cheméo Relay (1.0)
vc	0.584	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.96	J/mol×K	566.28	Joback Method
cpg	402.73	J/mol×K	595.54	Joback Method
cpg	414.96	J/mol×K	624.80	Joback Method
cpg	426.66	J/mol×K	654.06	Joback Method
cpg	437.84	J/mol×K	683.32	Joback Method
cpg	448.52	J/mol×K	712.57	Joback Method
cpg	458.70	J/mol×K	741.83	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=C26901973&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume