

2-ethylhexyl thioglycolate

Inchi:	InChI=1S/C10H20O2S/c1-3-5-6-9(4-2)7-12-10(11)8-13/h9,13H,3-8H2,1-2H3
InchiKey:	OWHSTLLOZWNTQ-UHFFFAOYSA-N
Formula:	C10H20O2S
SMILES:	CCCCC(CC)COC(=O)CS
Mol. weight [g/mol]:	204.34

Physical Properties

Property code	Value	Unit	Source
af	0.6421		Cheméo Relay (1.0)
hf	-554.33	kJ/mol	Cheméo Relay (1.0)
hfus	24.96	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.24		Cheméo Relay (1.0)
logp	2.676		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	524.21	K	Cheméo Relay (1.0)
tc	714.91	K	Cheméo Relay (1.0)
tf	202.86	K	Cheméo Relay (1.0)
vc	0.610	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.94	J/mol×K	566.91	Joback Method
cpg	437.78	J/mol×K	599.13	Joback Method
cpg	451.94	J/mol×K	631.34	Joback Method
cpg	465.43	J/mol×K	663.56	Joback Method
cpg	478.26	J/mol×K	695.77	Joback Method
cpg	490.44	J/mol×K	727.99	Joback Method
cpg	501.97	J/mol×K	760.21	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):	

Liquid-Liquid Equilibria for the Ternary Systems of Water + Thioglycolic Acid + 2-Ethyl-1-hexyl Thioglycolate and Water + 2-Ethyl-1-hexyl Thioglycolate + 2-Ethyl-1-hexanol at 293.15, 303.15, and 313.15 K under 101 kPa: <https://www.doi.org/10.1021/acs.jced.8b00619>

Legend

af:	Acentric Factor
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
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

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