

Ether, 2-[(2-methylallyl)thio]ethyl 2,6-xylyl

Inchi:	InChI=1S/C14H20OS/c1-11(2)10-16-9-8-15-14-12(3)6-5-7-13(14)4/h5-7H,1,8-10H2,2-4H
InchiKey:	QUZSXTKJJFGERC-UHFFFAOYSA-N
Formula:	C14H20OS
SMILES:	<chem>C=C(C)CSCCOc1c(C)cccc1C</chem>
Mol. weight [g/mol]:	236.37

Physical Properties

Property code	Value	Unit	Source
gf	167.56	kJ/mol	Joback Method
hf	-93.41	kJ/mol	Joback Method
hfus	28.01	kJ/mol	Joback Method
hvap	59.00	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.992		Crippen Method
mvol	202.280	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
tb	644.12	K	Joback Method
tc	862.33	K	Joback Method
tf	339.91	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.70	J/molxK	644.12	Joback Method
cpg	525.51	J/molxK	680.49	Joback Method
cpg	541.35	J/molxK	716.86	Joback Method
cpg	556.22	J/molxK	753.23	Joback Method
cpg	570.15	J/molxK	789.59	Joback Method
cpg	583.17	J/molxK	825.96	Joback Method
cpg	595.28	J/molxK	862.33	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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