(S)-3-Ethyl-4-methylpentanol

Other names: 3-Ethyl-4-methyl-1-pentanol
Inchi: InChI=1S/C8H18O/c1-4-8(5-6-9)7(2)3/h7-9H,4-6H2,1-3H3/t8-/m1/s1
InchiKey: RWIFVESHBHTZEM-MRVPVSSYSA-N
Formula: C8H18O
SMILES: CCC(CCO)C(C)C
Mol. weight [g/mol]: 130.23

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.051		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1020.10		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1020.10		NIST Webbook
rinpol	1008.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	473.74	K	Joback Method
tc	639.93	K	Joback Method
tf	210.74	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.39	J/mol×K	473.74	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	314.22	J/mol×K	529.14	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method
cpg	356.45	J/mol×K	639.93	Joback Method
dvisc	0.0001609	Pa×s	473.74	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=U144071&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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