

4-Heptanol, 4-ethyl-2,6-dimethyl-

Other names:	4-ethyl-2,6-dimethyl-4-heptanol
Inchi:	InChI=1S/C11H24O/c1-6-11(12,7-9(2)3)8-10(4)5/h9-10,12H,6-8H2,1-5H3
InchiKey:	FHFITCYHABMGHH-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCC(O)(CC(C)C)CC(C)C
Mol. weight [g/mol]:	172.31
CAS:	54460-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-97.12	kJ/mol	Joback Method
hf	-441.91	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.220		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
tb	539.15	K	Joback Method
tc	710.92	K	Joback Method
tf	246.97	K	Joback Method
vc	0.647	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.12	J/molxK	539.15	Joback Method
cpg	502.13	J/molxK	682.29	Joback Method
cpg	489.47	J/molxK	653.66	Joback Method
cpg	476.16	J/molxK	625.03	Joback Method
cpg	462.19	J/molxK	596.41	Joback Method
cpg	447.51	J/molxK	567.78	Joback Method
cpg	514.19	J/molxK	710.92	Joback Method
dvisc	0.0000871	Paxs	539.15	Joback Method

dvisc	0.0001625	Paxs	490.45	Joback Method
dvisc	0.0003474	Paxs	441.76	Joback Method
dvisc	0.0008970	Paxs	393.06	Joback Method
dvisc	0.0030283	Paxs	344.36	Joback Method
dvisc	0.0152643	Paxs	295.67	Joback Method
dvisc	0.1456070	Paxs	246.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54460990&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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