4-Heptanol, 2,6-dimethyl-4-(1-methylethyl)-

Inchi: InChI=1S/C12H26O/c1-9(2)7-12(13,11(5)6)8-10(3)4/h9-11,13H,7-8H2,1-6H3
InchiKey: MRVUYQAVPDEPRD-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CC(C)CC(O)(CC(C)C)C(C)C
Mol. weight [g/mol]: 186.33
CAS: 54775-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-91.14	kJ/mol	Joback Method
hf	-467.83	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.466		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
tb	561.59	K	Joback Method
tc	735.20	K	Joback Method
tf	243.24	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.19	J/mol×K	561.59	Joback Method
cpg	498.50	J/mol×K	590.52	Joback Method
cpg	514.02	J/mol×K	619.46	Joback Method
cpg	528.80	J/mol×K	648.39	Joback Method
cpg	542.87	J/mol×K	677.33	Joback Method
cpg	556.24	J/mol×K	706.26	Joback Method
cpg	568.96	J/mol×K	735.20	Joback Method
dvisc	0.2395481	Pa×s	243.24	Joback Method
dvisc	0.0180261	Pa×s	296.30	Joback Method

dvisc	0.0029763	Pa×s	349.36	Joback Method
dvisc	0.0007902	Pa×s	402.41	Joback Method
dvisc	0.0002857	Pa×s	455.47	Joback Method
dvisc	0.0001277	Pa×s	508.53	Joback Method
dvisc	0.0000665	Pa×s	561.59	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=C54775018&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
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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