

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/molxK	561.59	Joback Method
cpg	498.50	J/molxK	590.52	Joback Method
cpg	514.02	J/molxK	619.46	Joback Method
cpg	528.80	J/molxK	648.39	Joback Method
cpg	542.87	J/molxK	677.33	Joback Method
cpg	556.24	J/molxK	706.26	Joback Method
cpg	568.96	J/molxK	735.20	Joback Method
dvisc	0.2395481	Paxs	243.24	Joback Method
dvisc	0.0180261	Paxs	296.30	Joback Method

dvisc	0.0029763	Paxs	349.36	Joback Method
dvisc	0.0007902	Paxs	402.41	Joback Method
dvisc	0.0002857	Paxs	455.47	Joback Method
dvisc	0.0001277	Paxs	508.53	Joback Method
dvisc	0.0000665	Paxs	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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