

4-Methylpentyl 3-hydroxy-2-methylenebutanoate

Inchi:	InChI=1S/C11H20O3/c1-8(2)6-5-7-14-11(13)9(3)10(4)12/h8,10,12H,3,5-7H2,1-2,4H3
InchiKey:	HLNKZECEKFRDQV-UHFFFAOYSA-N
Formula:	C11H20O3
SMILES:	C=C(C(=O)OCCCC(C)C)C(C)O
Mol. weight [g/mol]:	200.27

Physical Properties

Property code	Value	Unit	Source
gf	-254.59	kJ/mol	Joback Method
hf	-562.32	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.903		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1387.90		NIST Webbook
rinpol	1387.90		NIST Webbook
tb	615.23	K	Joback Method
tc	791.51	K	Joback Method
tf	300.99	K	Joback Method
vc	0.664	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.65	J/mol×K	615.23	Joback Method
cpg	470.71	J/mol×K	644.61	Joback Method
cpg	483.18	J/mol×K	673.99	Joback Method
cpg	495.06	J/mol×K	703.37	Joback Method
cpg	506.38	J/mol×K	732.75	Joback Method
cpg	517.14	J/mol×K	762.13	Joback Method
cpg	527.35	J/mol×K	791.51	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=U413531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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