

Methyl dihydromalvalate

Inchi:	InChI=1S/C19H36O2/c1-3-4-5-6-7-10-13-17-16-18(17)14-11-8-9-12-15-19(20)21-2/h17-1
InchiKey:	LYLDBNFUPQGLCE-UHFFFAOYSA-N
Formula:	C19H36O2
SMILES:	CCCCCCCC1CC1CCCCCCC(=O)OC
Mol. weight [g/mol]:	296.49

Physical Properties

Property code	Value	Unit	Source
gf	-71.78	kJ/mol	Joback Method
hf	-627.83	kJ/mol	Joback Method
hfus	46.96	kJ/mol	Joback Method
hvap	66.65	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.887		Crippen Method
mvol	275.150	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	712.48	K	Joback Method
tc	887.77	K	Joback Method
tf	389.75	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.52	J/molxK	712.48	Joback Method
cpg	926.05	J/molxK	858.56	Joback Method
cpg	909.89	J/molxK	829.34	Joback Method
cpg	892.89	J/molxK	800.13	Joback Method
cpg	875.02	J/molxK	770.91	Joback Method
cpg	856.24	J/molxK	741.70	Joback Method
cpg	941.40	J/molxK	887.77	Joback Method
dvisc	0.0002816	Paxs	712.48	Joback Method

dvisc	0.0003424	Paxs	658.69	Joback Method
dvisc	0.0004309	Paxs	604.90	Joback Method
dvisc	0.0005673	Paxs	551.12	Joback Method
dvisc	0.0007926	Paxs	497.33	Joback Method
dvisc	0.0012010	Paxs	443.54	Joback Method
dvisc	0.0020409	Paxs	389.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R287575&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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