

1-p-Menthen-9-yl 3-methylbutanoate

Inchi:	InChI=1S/C15H26O2/c1-11(2)9-15(16)17-10-13(4)14-7-5-12(3)6-8-14/h5,11,13-14H,6-10
InchiKey:	VJJQDACGAQKNSG-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CC1=CCC(C(C)COC(=O)CC(C)C)CC1
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-118.60	kJ/mol	Joback Method
hf	-507.66	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.958		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	641.70	K	Joback Method
tc	843.11	K	Joback Method
tf	321.63	K	Joback Method
vc	0.806	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.61	J/molxK	641.70	Joback Method
cpg	682.31	J/molxK	809.54	Joback Method
cpg	666.68	J/molxK	775.97	Joback Method
cpg	650.01	J/molxK	742.41	Joback Method
cpg	632.29	J/molxK	708.84	Joback Method
cpg	613.50	J/molxK	675.27	Joback Method
cpg	696.94	J/molxK	843.11	Joback Method
dvisc	0.0001290	Paxs	641.70	Joback Method
dvisc	0.0001746	Paxs	588.36	Joback Method

dvisc	0.0002511	Paxs	535.01	Joback Method
dvisc	0.0003913	Paxs	481.67	Joback Method
dvisc	0.0006813	Paxs	428.32	Joback Method
dvisc	0.0013886	Paxs	374.98	Joback Method
dvisc	0.0035846	Paxs	321.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R589425&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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