

MENTHOL, O-ISOBUTENYRYL-

Other names:	Menthyl methacrylate
Inchi:	InChI=1S/C14H24O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h9,11-13H,3,6-8H2,1-
InchiKey:	VYPRXWXGLLURNB-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	C=C(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
hfus	22.67	kJ/mol	Joback Method
hvap	70.39	kJ/mol	Cheméo Relay (1.0)
logp	3.567		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	524.97	K	Cheméo Relay (1.0)
tc	728.60	K	Cheméo Relay (1.0)
tf	244.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.26	J/mol×K	602.34	Joback Method
cpg	561.38	J/mol×K	636.44	Joback Method
cpg	581.36	J/mol×K	670.55	Joback Method
cpg	600.23	J/mol×K	704.65	Joback Method
cpg	618.00	J/mol×K	738.76	Joback Method
cpg	634.69	J/mol×K	772.86	Joback Method
cpg	650.30	J/mol×K	806.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U127500&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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