

2-Methylallyl methacrylate

Inchi:	InChI=1S/C8H12O2/c1-6(2)5-10-8(9)7(3)4/h1,3,5H2,2,4H3
InchiKey:	TVBLIEXOPWWREN-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	C=C(C)COC(=O)C(=C)C
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
hf	-302.50	kJ/mol	Cheméo Relay (1.0)
hfus	14.08	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	1.682		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
tb	428.70	K	Cheméo Relay (1.0)
tf	242.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.48	J/mol×K	451.85	Joback Method
cpg	257.84	J/mol×K	483.38	Joback Method
cpg	268.71	J/mol×K	514.92	Joback Method
cpg	279.10	J/mol×K	546.45	Joback Method
cpg	289.02	J/mol×K	577.99	Joback Method
cpg	298.48	J/mol×K	609.52	Joback Method
cpg	307.49	J/mol×K	641.06	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C816740&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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