

3-Methyl-2-butenolic acid, 3-methylbutyl ester

Other names:	3-Methyl-2-butenolic acid, 3-methylbutyl ester 3-methylbutyl 3-methylbut-2-enoate isopentyl 3-methyl-2-butenolate
Inchi:	InChI=1S/C10H18O2/c1-8(2)5-6-12-10(11)7-9(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	DBGLRAHCYJTYEH-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)=CC(=O)OCCC(C)C
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
hf	-477.04	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.14		Cheméo Relay (1.0)
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1184.00		NIST Webbook
tb	471.23	K	Cheméo Relay (1.0)
tc	656.97	K	Cheméo Relay (1.0)
tf	221.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.82	J/mol×K	508.09	Joback Method
cpg	365.21	J/mol×K	539.21	Joback Method
cpg	378.95	J/mol×K	570.33	Joback Method
cpg	392.08	J/mol×K	601.46	Joback Method
cpg	404.60	J/mol×K	632.58	Joback Method

cpg	416.53	J/mol×K	663.70	Joback Method
cpg	427.88	J/mol×K	694.82	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56922737&Units=SI

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
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

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