3-Methylpentyl methacrylate

Inchi:	InChI=1S/C10H18O2/c1-5-9(4)6-7-12-10(11)8(2)3/h9H,2,5-7H2,1,3-4H3
InchiKey:	QKMOBSUDXQCKPG-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=C(C)C(=O)OCCC(C)CC
Mol. weight [g/mol]:	170.25
CAS:	113615-00-2

Physical Properties

Property code	Value	Unit	Source
gf	-123.75	kJ/mol	Joback Method
hf	-384.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1147.70		NIST Webbook
rinpol	1147.70		NIST Webbook
tb	500.61	K	Joback Method
tc	682.86	K	Joback Method
tf	243.90	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.92	J/mol×K	500.61	Joback Method
cpg	364.09	J/mol×K	530.98	Joback Method
cpg	377.66	J/mol×K	561.36	Joback Method
cpg	390.66	J/mol×K	591.73	Joback Method
cpg	403.09	J/mol×K	622.11	Joback Method
cpg	414.96	J/mol×K	652.48	Joback Method
cpg	426.29	J/mol×K	682.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113615002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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