

Methacrylic acid, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C12H14O2/c1-8(2)12(13)14-11-7-5-6-9(3)10(11)4/h5-7H,1H2,2-4H3
InchiKey:	PDRUPOCQIPHOB-LUHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	C=C(C)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
gf	-11.32	kJ/mol	Joback Method
hf	-206.58	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.785		Crippen Method
mvol	159.320	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1448.00		NIST Webbook
tb	583.45	K	Joback Method
tc	799.42	K	Joback Method
tf	332.90	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.75	J/molxK	583.45	Joback Method
cpg	386.99	J/molxK	619.45	Joback Method
cpg	400.43	J/molxK	655.44	Joback Method
cpg	413.11	J/molxK	691.44	Joback Method
cpg	425.02	J/molxK	727.43	Joback Method
cpg	436.20	J/molxK	763.43	Joback Method
cpg	446.66	J/molxK	799.42	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=U360692&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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