

Mesitylacetic acid

Other names:	2-Mesityleneacetic acid Benzeneacetic acid, 2,4,6-trimethyl- (2,4,6-trimethylphenyl)acetic acid
Inchi:	InChI=1S/C11H14O2/c1-7-4-8(2)10(6-11(12)13)9(3)5-7/h4-5H,6H2,1-3H3,(H,12,13)
InchiKey:	CQWMQAKKAHTCSC-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	<chem>Cc1cc(C)c(CC(=O)O)c(C)c1</chem>
Mol. weight [g/mol]:	178.23
CAS:	4408-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-140.48	kJ/mol	Joback Method
hf	-333.06	kJ/mol	Joback Method
hfus	22.81	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.239		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
tb	638.75	K	Joback Method
tc	839.03	K	Joback Method
tf	388.46	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.60	J/molxK	638.75	Joback Method
cpg	424.01	J/molxK	805.65	Joback Method
cpg	414.88	J/molxK	772.27	Joback Method
cpg	405.19	J/molxK	738.89	Joback Method
cpg	394.92	J/molxK	705.51	Joback Method
cpg	384.06	J/molxK	672.13	Joback Method

cpg	432.59	J/mol×K	839.03	Joback Method
dvisc	0.0000718	Paxs	638.75	Joback Method
dvisc	0.0001018	Paxs	597.04	Joback Method
dvisc	0.0001522	Paxs	555.32	Joback Method
dvisc	0.0002427	Paxs	513.61	Joback Method
dvisc	0.0004203	Paxs	471.89	Joback Method
dvisc	0.0008099	Paxs	430.18	Joback Method
dvisc	0.0017966	Paxs	388.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4408600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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