

Benzeneacetic acid, «alpha»-ethyl-, methyl ester

Other names:	Butyric acid, 2-phenyl-, methyl ester Methyl «alpha»-phenylbutyrate Methyl 2-phenylbutyrate (. +/-)-2-Phenylbutyric acid, methyl ester Methyl 2-phenylbutanoate
Inchi:	InChI=1S/C11H14O2/c1-3-10(11(12)13-2)9-7-5-4-6-8-9/h4-8,10H,3H2,1-2H3
InchiKey:	PPIQQNDMGXNRFA-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCC(C(=O)OC)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	2294-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-82.21	kJ/mol	Joback Method
hf	-283.92	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.353		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1287.10		NIST Webbook
rinpol	1287.30		NIST Webbook
tb	553.61	K	Joback Method
tc	767.42	K	Joback Method
tf	297.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.73	J/molxK	553.61	Joback Method
cpg	412.55	J/molxK	731.79	Joback Method

cpg	401.00	J/mol×K	696.15	Joback Method
cpg	388.67	J/mol×K	660.52	Joback Method
cpg	375.53	J/mol×K	624.88	Joback Method
cpg	361.56	J/mol×K	589.25	Joback Method
cpg	423.32	J/mol×K	767.42	Joback Method
dvisc	0.0001883	Paxs	553.61	Joback Method
dvisc	0.0002466	Paxs	510.89	Joback Method
dvisc	0.0003393	Paxs	468.18	Joback Method
dvisc	0.0004976	Paxs	425.46	Joback Method
dvisc	0.0007949	Paxs	382.74	Joback Method
dvisc	0.0014284	Paxs	340.03	Joback Method
dvisc	0.0030377	Paxs	297.31	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=C2294715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
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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