4-(1-Carboxyethyl)benzoic acid, dimethyl

Inchi: InChI=1S/C12H14O4/c1-8(11(13)15-2)9-4-6-10(7-5-9)12(14)16-3/h4-8H,1-3H3
InchiKey: LMGDXEZEUHTSEE-UHFFFAOYSA-N
Formula: C12H14O4
SMILES: COC(=O)c1ccc(C(C)C(=O)OC)cc1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	-317.34	kJ/mol	Joback Method
hf	-560.83	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.750		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1618.00		NIST Webbook
tb	657.76	K	Joback Method
tc	873.64	K	Joback Method
tf	393.26	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.03	J/mol×K	657.76	Joback Method
cpg	450.66	J/mol×K	693.74	Joback Method
cpg	463.45	J/mol×K	729.72	Joback Method
cpg	475.39	J/mol×K	765.70	Joback Method
cpg	486.48	J/mol×K	801.68	Joback Method
cpg	496.72	J/mol×K	837.66	Joback Method
cpg	506.12	J/mol×K	873.64	Joback Method
dvisc	0.0013098	Pa×s	393.26	Joback Method
dvisc	0.0007459	Pa×s	437.34	Joback Method

dvisc	0.0004709	Pa×s	481.43	Joback Method
dvisc	0.0003211	Pa×s	525.51	Joback Method
dvisc	0.0002323	Pa×s	569.59	Joback Method
dvisc	0.0001761	Pa×s	613.68	Joback Method
dvisc	0.0001386	Pa×s	657.76	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=R399534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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