O-(carboxymethoxy) benzoic acid

Inchi: InChI=1S/C9H8O5/c10-8(11)5-14-7-4-2-1-3-6(7)9(12)13/h1-4H,5H2,(H,10,11)(H,12,13)
InchiKey: JLLXSRLEXBECPY-UHFFFAOYSA-N
Formula: C9H8O5
SMILES: O=C(O)COc1ccccc1C(=O)O
Mol. weight [g/mol]: 196.16
CAS: 635-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-508.80	kJ/mol	Joback Method
hf	-665.87	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	87.83	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.848		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	751.50	K	Joback Method
tc	950.28	K	Joback Method
tf	473.86	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.80	J/mol×K	751.50	Joback Method
cpg	361.08	J/mol×K	784.63	Joback Method
cpg	367.83	J/mol×K	817.76	Joback Method
cpg	374.07	J/mol×K	850.89	Joback Method
cpg	379.79	J/mol×K	884.02	Joback Method
cpg	385.02	J/mol×K	917.15	Joback Method
cpg	389.75	J/mol×K	950.28	Joback Method
dvisc	0.0006454	Pa×s	473.86	Joback Method
dvisc	0.0002434	Pa×s	520.13	Joback Method

dvisc	0.0001077	Pa×s	566.41	Joback Method
dvisc	0.0000539	Pa×s	612.68	Joback Method
dvisc	0.0000297	Pa×s	658.95	Joback Method
dvisc	0.0000177	Pa×s	705.23	Joback Method
dvisc	0.0000113	Pa×s	751.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C635530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:
https://www.chemeo.com/cid/66-719-1/O-carboxymethoxy-benzoic-acid.pdf
Generated by Cheméo on 2024-04-20 14:27:05.541132447 +0000 UTC m=+15912474.461709760.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.