Diallyl malonate

Inchi: InChI=1S/C9H12O4/c1-3-5-12-8(10)7-9(11)13-6-4-2/h3-4H,1-2,5-7H2
InchiKey: AOESAXAWXYJFNC-UHFFFAOYSA-N
Formula: C9H12O4
SMILES: C=CCOC(=O)CC(=O)OCC=C
Mol. weight [g/mol]: 184.19

Physical Properties

Property code	Value	Unit	Source
gf	-267.26	kJ/mol	Joback Method
hf	-467.83	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	0.835		Crippen Method
mcvol	143.950	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1178.00		NIST Webbook
tb	551.26	K	Joback Method
tc	739.86	K	Joback Method
tf	331.99	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.13	J/mol×K	551.26	Joback Method
cpg	340.24	J/mol×K	582.69	Joback Method
cpg	350.85	J/mol×K	614.13	Joback Method
cpg	360.99	J/mol×K	645.56	Joback Method
cpg	370.63	J/mol×K	676.99	Joback Method
cpg	379.79	J/mol×K	708.42	Joback Method
cpg	388.46	J/mol×K	739.86	Joback Method
dvisc	0.0018303	Pa×s	331.99	Joback Method
dvisc	0.0010807	Pa×s	368.54	Joback Method

dvisc	0.0007017	Pa×s	405.08	Joback Method
dvisc	0.0004894	Pa×s	441.62	Joback Method
dvisc	0.0003606	Pa×s	478.17	Joback Method
dvisc	0.0002775	Pa×s	514.71	Joback Method
dvisc	0.0002211	Pa×s	551.26	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=R542317&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