

Diethyl, allyl-(1-ethylpropyl) malonate

Inchi:	InChI=1S/C15H26O4/c1-6-11-15(12(7-2)8-3,13(16)18-9-4)14(17)19-10-5/h6,12H,1,7-11H
InchiKey:	NUEFNOFCCKXHOY-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	<chem>C=CCC(C(=O)OCC)(C(=O)OCC)C(CC)CC</chem>
Mol. weight [g/mol]:	270.36
CAS:	101107-08-8

Physical Properties

Property code	Value	Unit	Source
gf	-304.18	kJ/mol	Joback Method
hf	-731.13	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.111		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
tb	688.19	K	Joback Method
tc	875.24	K	Joback Method
tf	388.79	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.30	J/molxK	688.19	Joback Method
cpg	672.53	J/molxK	719.37	Joback Method
cpg	687.88	J/molxK	750.54	Joback Method
cpg	702.36	J/molxK	781.72	Joback Method
cpg	716.02	J/molxK	812.89	Joback Method
cpg	728.86	J/molxK	844.07	Joback Method
cpg	740.91	J/molxK	875.24	Joback Method
dvisc	0.0017327	Paxs	388.79	Joback Method
dvisc	0.0007928	Paxs	438.69	Joback Method

dvisc	0.0004255	Paxs	488.59	Joback Method
dvisc	0.0002563	Paxs	538.49	Joback Method
dvisc	0.0001683	Paxs	588.39	Joback Method
dvisc	0.0001180	Paxs	638.29	Joback Method
dvisc	0.0000871	Paxs	688.19	Joback Method

Sources

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=C101107088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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