Diethylmalonic acid, butyl 2-methoxyethyl ester

Inchi: InChI=1S/C14H26O5/c1-5-8-9-18-12(15)14(6-2,7-3)13(16)19-11-10-17-4/h5-11H2,1-4H3

InchiKey: IPNAFPSIXXUZMK-UHFFFAOYSA-N

Formula: C14H26O5

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OCCOC

Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-503.00	kJ/mol	Joback Method
hf	-962.86	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.326		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	1600.00		NIST Webbook
tb	691.49	K	Joback Method
tc	874.22	K	Joback Method
tf	416.51	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.43	J/mol×K	691.49	Joback Method
cpg	724.35	J/mol×K	843.76	Joback Method
cpg	711.78	J/mol×K	813.31	Joback Method
cpg	698.40	J/mol×K	782.85	Joback Method
cpg	684.23	J/mol×K	752.40	Joback Method
cpg	669.24	J/mol×K	721.94	Joback Method
cpg	736.14	J/mol×K	874.22	Joback Method
dvisc	0.0000777	Pa×s	691.49	Joback Method
dvisc	0.0001028	Pa×s	645.66	Joback Method

dvisc	0.0001420	Pa×s	599.83	Joback Method
dvisc	0.0002068	Pa×s	554.00	Joback Method
dvisc	0.0003225	Pa×s	508.17	Joback Method
dvisc	0.0005490	Pa×s	462.34	Joback Method
dvisc	0.0010508	Pa×s	416.51	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=U370672&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