Propanedioic acid, methyl-, dibutyl ester

Other names: Dibutyl-2-methylmalonate
Inchi: InChI=1S/C12H22O4/c1-4-6-8-15-11(13)10(3)12(14)16-9-7-5-2/h10H,4-9H2,1-3H3
InchiKey: PYKIHPRFFNLVMF-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CCCCOC(=O)C(C)C(=O)OCCCC
Mol. weight [g/mol]: 230.30
CAS: 52886-83-6

Physical Properties

Property code	Value	Unit	Source
gf	-420.12	kJ/mol	Joback Method
hf	-785.89	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.309		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	626.10	K	Joback Method
tc	806.33	K	Joback Method
tf	354.32	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.38	J/mol×K	626.10	Joback Method
cpg	531.21	J/mol×K	656.14	Joback Method
cpg	545.37	J/mol×K	686.18	Joback Method
cpg	558.88	J/mol×K	716.21	Joback Method
cpg	571.72	J/mol×K	746.25	Joback Method
cpg	583.91	J/mol×K	776.29	Joback Method

cpg	595.44	J/mol×K	806.33	Joback Method
dvisc	0.0021379	Pa×s	354.32	Joback Method
dvisc	0.0010527	Pa×s	399.62	Joback Method
dvisc	0.0005987	Pa×s	444.91	Joback Method
dvisc	0.0003780	Pa×s	490.21	Joback Method
dvisc	0.0002579	Pa×s	535.51	Joback Method
dvisc	0.0001868	Pa×s	580.80	Joback Method
dvisc	0.0001418	Pa×s	626.10	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52886836&Units=SI

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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