Succinic acid, 3-methylbut-2-yl 2-methoxyethyl ester

Inchi: InChI=1S/C12H22O5/c1-9(2)10(3)17-12(14)6-5-11(13)16-8-7-15-4/h9-10H,5-8H2,1-4H3

InchiKey: KWGDYNAFAFLTHI-UHFFFAOYSA-N

Formula: C12H22O5

SMILES: COCCOC(=O)CCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
gf	-527.56	kJ/mol	Joback Method
hf	-923.39	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.544		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1580.00		NIST Webbook
tb	648.08	K	Joback Method
tc	830.65	K	Joback Method
tf	361.55	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.21	J/mol×K	648.08	Joback Method
cpg	559.13	J/mol×K	678.51	Joback Method
cpg	573.35	J/mol×K	708.94	Joback Method
cpg	586.88	J/mol×K	739.36	Joback Method
cpg	599.71	J/mol×K	769.79	Joback Method
cpg	611.82	J/mol×K	800.22	Joback Method
cpg	623.21	J/mol×K	830.65	Joback Method
dvisc	0.0018669	Pa×s	361.55	Joback Method
dvisc	0.0008676	Pa×s	409.31	Joback Method

dvisc	0.0004732	Pa×s	457.06	Joback Method
dvisc	0.0002895	Pa×s	504.81	Joback Method
dvisc	0.0001928	Pa×s	552.57	Joback Method
dvisc	0.0001370	Pa×s	600.32	Joback Method
dvisc	0.0001023	Pa×s	648.08	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=U390734&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