Succinic acid, 3-methylbut-2-en-1-yl 2-methoxyethyl ester

Inchi: InChI=1S/C12H20O5/c1-10(2)6-7-16-11(13)4-5-12(14)17-9-8-15-3/h6H,4-5,7-9H2,1-3H3

InchiKey: HTHHIMNSGQPEOB-UHFFFAOYSA-N

Formula: C12H20O5

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

Mol. weight [g/mol]: 244.28

Physical Properties

Property code	Value	Unit	Source
gf	-451.01	kJ/mol	Joback Method
hf	-805.40	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.466		Crippen Method
mcvol	196.390	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1687.00		NIST Webbook
tb	653.00	K	Joback Method
tc	838.36	K	Joback Method
tf	372.51	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.43	J/mol×K	653.00	Joback Method
cpg	535.49	J/mol×K	683.89	Joback Method
cpg	548.89	J/mol×K	714.79	Joback Method
cpg	561.62	J/mol×K	745.68	Joback Method
cpg	573.68	J/mol×K	776.58	Joback Method
cpg	585.08	J/mol×K	807.47	Joback Method
cpg	595.81	J/mol×K	838.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390736&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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