Succinic acid, isobutyl 3-methoxybenzyl ester

Inchi: InChI=1S/C16H22O5/c1-12(2)10-20-15(17)7-8-16(18)21-11-13-5-4-6-14(9-13)19-3/h4-6,
InchiKey: DXEKQEAEVTZGDK-UHFFFAOYSA-N
Formula: C16H22O5
SMILES: COc1cccc(COC(=O)CCC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-388.66	kJ/mol	Joback Method
hf	-775.61	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.718		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	771.70	K	Joback Method
tc	975.50	K	Joback Method
tf	460.57	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.85	J/mol×K	771.70	Joback Method
cpg	691.80	J/mol×K	805.67	Joback Method
cpg	705.71	J/mol×K	839.63	Joback Method
cpg	718.58	J/mol×K	873.60	Joback Method
cpg	730.40	J/mol×K	907.57	Joback Method
cpg	741.18	J/mol×K	941.54	Joback Method
cpg	750.92	J/mol×K	975.50	Joback Method
dvisc	0.0006944	Pa×s	460.57	Joback Method

dvisc	0.0003841	Pa×s	512.42	Joback Method
dvisc	0.0002368	Pa×s	564.28	Joback Method
dvisc	0.0001584	Pa×s	616.13	Joback Method
dvisc	0.0001128	Pa×s	667.99	Joback Method
dvisc	0.0000844	Pa×s	719.85	Joback Method
dvisc	0.0000656	Pa×s	771.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381252&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

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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