Sebacic acid, isobutyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C19H36O4/c1-15(2)14-22-18(20)12-10-8-6-7-9-11-13-19(21)23-17(5)16(3)4/h1
InchiKey: XYQJYLFRRUEMGA-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-366.06	kJ/mol	Joback Method
hf	-940.93	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.894		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	785.38	K	Joback Method
tc	969.72	K	Joback Method
tf	403.21	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.35	J/mol×K	785.38	Joback Method
cpg	928.54	J/mol×K	816.10	Joback Method
cpg	945.69	J/mol×K	846.83	Joback Method
cpg	961.82	J/mol×K	877.55	Joback Method
cpg	976.93	J/mol×K	908.28	Joback Method
cpg	991.06	J/mol×K	939.00	Joback Method
cpg	1004.20	J/mol×K	969.72	Joback Method
dvisc	0.0016792	Pa×s	403.21	Joback Method

dvisc	0.0006190	Pa×s	466.90	Joback Method
dvisc	0.0002900	Pa×s	530.60	Joback Method
dvisc	0.0001598	Pa×s	594.29	Joback Method
dvisc	0.0000989	Pa×s	657.99	Joback Method
dvisc	0.0000666	Pa×s	721.68	Joback Method
dvisc	0.0000478	Pa×s	785.38	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=U355559&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