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

Inchi: InChI=1S/C20H38O4/c1-16(2)15-23-18(21)13-11-9-7-8-10-12-14-19(22)24-17(3)20(4,5)6
InchiKey: LKTCPSXTSMOLTL-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-352.36	kJ/mol	Joback Method
hf	-965.04	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.284		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2211.00		NIST Webbook
tb	805.47	K	Joback Method
tc	993.66	K	Joback Method
tf	431.90	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.15	J/mol×K	805.47	Joback Method
cpg	989.61	J/mol×K	836.83	Joback Method
cpg	1006.98	J/mol×K	868.20	Joback Method
cpg	1023.29	J/mol×K	899.56	Joback Method
cpg	1038.57	J/mol×K	930.93	Joback Method
cpg	1052.84	J/mol×K	962.29	Joback Method
cpg	1066.15	J/mol×K	993.66	Joback Method
dvisc	0.0011766	Pa×s	431.90	Joback Method
dvisc	0.0004564	Pa×s	494.16	Joback Method

dvisc	0.0002188	Pa×s	556.42	Joback Method
dvisc	0.0001216	Pa×s	618.68	Joback Method
dvisc	0.0000753	Pa×s	680.95	Joback Method
dvisc	0.0000505	Pa×s	743.21	Joback Method
dvisc	0.0000360	Pa×s	805.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355596&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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