

Sebacic acid, di(3-methylbut-2-yl) ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-360.08	kJ/mol	Joback Method
hf	-966.85	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.283		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinsol	2231.00		NIST Webbook
tb	807.82	K	Joback Method
tc	995.23	K	Joback Method
tf	399.48	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.09	J/molxK	807.82	Joback Method
cpg	1053.20	J/molxK	963.99	Joback Method
cpg	1038.95	J/molxK	932.76	Joback Method
cpg	1023.63	J/molxK	901.52	Joback Method
cpg	1007.22	J/molxK	870.29	Joback Method
cpg	989.72	J/molxK	839.05	Joback Method
cpg	1066.41	J/molxK	995.23	Joback Method
dvisc	0.0000379	Paxs	807.82	Joback Method
dvisc	0.0000538	Paxs	739.76	Joback Method

dvisc	0.0000821	Paxs	671.71	Joback Method
dvisc	0.0001376	Paxs	603.65	Joback Method
dvisc	0.0002633	Paxs	535.59	Joback Method
dvisc	0.0006083	Paxs	467.54	Joback Method
dvisc	0.0018698	Paxs	399.48	Joback Method

Sources

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=U355574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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