

Sebacic acid, isobutyl 2-methylphenyl ester

Inchi:	InChI=1S/C21H32O4/c1-17(2)16-24-20(22)14-8-6-4-5-7-9-15-21(23)25-19-13-11-10-12-
InchiKey:	MYHKHEXPGVVRTN-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	<chem>Cc1ccccc1OC(=O)CCCCCCCCC(=O)OCC(C)C</chem>
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-241.56	kJ/mol	Joback Method
hf	-746.59	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.220		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinpola	2592.00		NIST Webbook
tb	863.68	K	Joback Method
tc	1066.32	K	Joback Method
tf	494.69	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.65	J/molxK	863.68	Joback Method
cpg	954.09	J/molxK	897.45	Joback Method
cpg	969.33	J/molxK	931.23	Joback Method
cpg	983.39	J/molxK	965.00	Joback Method
cpg	996.30	J/molxK	998.77	Joback Method
cpg	1008.08	J/molxK	1032.54	Joback Method
cpg	1018.76	J/molxK	1066.32	Joback Method
dvisc	0.0006043	Paxs	494.69	Joback Method
dvisc	0.0003060	Paxs	556.19	Joback Method

dvisc	0.0001775	Paxs	617.69	Joback Method
dvisc	0.0001136	Paxs	679.18	Joback Method
dvisc	0.0000783	Paxs	740.68	Joback Method
dvisc	0.0000571	Paxs	802.18	Joback Method
dvisc	0.0000436	Paxs	863.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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