

Sebacic acid, 3,4-dimethylphenyl isobutyl ester

Inchi:	InChI=1S/C22H34O4/c1-17(2)16-25-21(23)11-9-7-5-6-8-10-12-22(24)26-20-14-13-18(3)
InchiKey:	MJMCNRCPHHJGAD-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	<chem>Cc1ccc(OC(=O)CCCCCCCC(=O)OCC(C)C)cc1C</chem>
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-242.77	kJ/mol	Joback Method
hf	-778.70	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.529		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinqol	2750.00		NIST Webbook
tb	891.54	K	Joback Method
tc	1096.74	K	Joback Method
tf	518.48	K	Joback Method
vc	1.202	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.20	J/molxK	891.54	Joback Method
cpg	1067.43	J/molxK	1062.54	Joback Method
cpg	1055.82	J/molxK	1028.34	Joback Method
cpg	1043.02	J/molxK	994.14	Joback Method
cpg	1029.00	J/molxK	959.94	Joback Method
cpg	1013.73	J/molxK	925.74	Joback Method
cpg	1077.87	J/molxK	1096.74	Joback Method
dvisc	0.0000384	Paxs	891.54	Joback Method
dvisc	0.0000497	Paxs	829.36	Joback Method

dvisc	0.0000673	Paxs	767.19	Joback Method
dvisc	0.0000959	Paxs	705.01	Joback Method
dvisc	0.0001465	Paxs	642.83	Joback Method
dvisc	0.0002450	Paxs	580.66	Joback Method
dvisc	0.0004636	Paxs	518.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354578&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

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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