

Sebacic acid, isobutyl 2-methylbenzyl ester

Inchi:	InChI=1S/C22H34O4/c1-18(2)16-25-21(23)14-8-6-4-5-7-9-15-22(24)26-17-20-13-11-10-
InchiKey:	FMYVHSSQJDZBDH-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	<chem>Cc1ccccc1COC(=O)CCCCCCCCC(=O)OCC(C)C</chem>
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-233.14	kJ/mol	Joback Method
hf	-767.23	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.358		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2628.00		NIST Webbook
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tb	886.56	K	Joback Method
tc	1090.83	K	Joback Method
tf	505.96	K	Joback Method
vc	1.202	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.77	J/molxK	886.56	Joback Method
cpg	1014.40	J/molxK	920.61	Joback Method
cpg	1029.77	J/molxK	954.65	Joback Method
cpg	1043.91	J/molxK	988.70	Joback Method
cpg	1056.86	J/molxK	1022.74	Joback Method
cpg	1068.64	J/molxK	1056.79	Joback Method
cpg	1079.28	J/molxK	1090.83	Joback Method
dvisc	0.0005411	Paxs	505.96	Joback Method

dvisc	0.0002711	Paxs	569.39	Joback Method
dvisc	0.0001560	Paxs	632.83	Joback Method
dvisc	0.0000993	Paxs	696.26	Joback Method
dvisc	0.0000682	Paxs	759.69	Joback Method
dvisc	0.0000496	Paxs	823.13	Joback Method
dvisc	0.0000377	Paxs	886.56	Joback Method

Sources

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=U380714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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