

Sebacic acid, isohexyl 2-methylphenyl ester

Inchi:	InChI=1S/C23H36O4/c1-19(2)13-12-18-26-22(24)16-8-6-4-5-7-9-17-23(25)27-21-15-11-
InchiKey:	QWMODGHVQCYLRW-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	Cc1ccccc1OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-224.72	kJ/mol	Joback Method
hf	-787.87	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.001		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinsol	2798.00		NIST Webbook
tb	909.44	K	Joback Method
tc	1116.16	K	Joback Method
tf	517.23	K	Joback Method
vc	1.258	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.53	J/molxK	909.44	Joback Method
cpg	1129.80	J/molxK	1081.71	Joback Method
cpg	1118.04	J/molxK	1047.26	Joback Method
cpg	1105.07	J/molxK	1012.80	Joback Method
cpg	1090.85	J/molxK	978.35	Joback Method
cpg	1075.35	J/molxK	943.89	Joback Method
cpg	1140.38	J/molxK	1116.16	Joback Method
dvisc	0.0000326	Paxs	909.44	Joback Method
dvisc	0.0000429	Paxs	844.07	Joback Method

dvisc	0.0000592	Paxs	778.70	Joback Method
dvisc	0.0000866	Paxs	713.34	Joback Method
dvisc	0.0001368	Paxs	647.97	Joback Method
dvisc	0.0002394	Paxs	582.60	Joback Method
dvisc	0.0004827	Paxs	517.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354375&Units=SI

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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