

Sebacic acid, hexyl 3-methylphenyl ester

Inchi:	InChI=1S/C23H36O4/c1-3-4-5-12-18-26-22(24)16-10-8-6-7-9-11-17-23(25)27-21-15-13-
InchiKey:	NTIXOHOSPCBQQU-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-222.28	kJ/mol	Joback Method
hf	-782.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.145		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2859.00		NIST Webbook
tb	909.88	K	Joback Method
tc	1115.88	K	Joback Method
tf	532.23	K	Joback Method
vc	1.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.08	J/molxK	909.88	Joback Method
cpg	1074.86	J/molxK	944.21	Joback Method
cpg	1090.35	J/molxK	978.55	Joback Method
cpg	1104.59	J/molxK	1012.88	Joback Method
cpg	1117.59	J/molxK	1047.21	Joback Method
cpg	1129.40	J/molxK	1081.55	Joback Method
cpg	1140.05	J/molxK	1115.88	Joback Method
dvisc	0.0004311	Paxs	532.23	Joback Method
dvisc	0.0002285	Paxs	595.17	Joback Method

dvisc	0.0001367	Paxs	658.11	Joback Method
dvisc	0.0000895	Paxs	721.06	Joback Method
dvisc	0.0000627	Paxs	784.00	Joback Method
dvisc	0.0000463	Paxs	846.94	Joback Method
dvisc	0.0000357	Paxs	909.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354928&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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