

Succinic acid, 2,3-dimethylphenyl undecyl ester

Inchi:	InChI=1S/C23H36O4/c1-4-5-6-7-8-9-10-11-12-18-26-22(24)16-17-23(25)27-21-15-13-14
InchiKey:	AHQFXSWPQCOFMG-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)Oc1ccc(C)c1C
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-231.91	kJ/mol	Joback Method
hf	-794.06	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.063		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	914.86	K	Joback Method
tc	1121.86	K	Joback Method
tf	544.75	K	Joback Method
vc	1.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.52	J/molxK	914.86	Joback Method
cpg	1074.21	J/molxK	949.36	Joback Method
cpg	1089.60	J/molxK	983.86	Joback Method
cpg	1103.70	J/molxK	1018.36	Joback Method
cpg	1116.54	J/molxK	1052.86	Joback Method
cpg	1128.16	J/molxK	1087.36	Joback Method
cpg	1138.58	J/molxK	1121.86	Joback Method
dvisc	0.0003755	Paxs	544.75	Joback Method

dvisc	0.0002088	Paxs	606.43	Joback Method
dvisc	0.0001294	Paxs	668.12	Joback Method
dvisc	0.0000869	Paxs	729.80	Joback Method
dvisc	0.0000621	Paxs	791.49	Joback Method
dvisc	0.0000466	Paxs	853.17	Joback Method
dvisc	0.0000364	Paxs	914.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349626&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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