

Sebacic acid, 2,3-dimethylphenyl ethyl ester

Inchi:	InChI=1S/C20H30O4/c1-4-23-19(21)14-9-7-5-6-8-10-15-20(22)24-18-13-11-12-16(2)17(
InchiKey:	CRGYPJGRJWEOECR-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-257.17	kJ/mol	Joback Method
hf	-732.14	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.893		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinqol	2537.00		NIST Webbook
tb	846.22	K	Joback Method
tc	1047.10	K	Joback Method
tf	510.94	K	Joback Method
vc	1.095	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.09	J/molxK	846.22	Joback Method
cpg	893.13	J/molxK	879.70	Joback Method
cpg	908.05	J/molxK	913.18	Joback Method
cpg	921.85	J/molxK	946.66	Joback Method
cpg	934.55	J/molxK	980.14	Joback Method
cpg	946.18	J/molxK	1013.62	Joback Method
cpg	956.74	J/molxK	1047.10	Joback Method
dvisc	0.0005107	Paxs	510.94	Joback Method
dvisc	0.0002940	Paxs	566.82	Joback Method

dvisc	0.0001869	Paxs	622.70	Joback Method
dvisc	0.0001280	Paxs	678.58	Joback Method
dvisc	0.0000929	Paxs	734.46	Joback Method
dvisc	0.0000705	Paxs	790.34	Joback Method
dvisc	0.0000555	Paxs	846.22	Joback Method

Sources

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=U355204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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