Sebacic acid, di(3,4-dimethylphenyl) ester

Inchi: InChI=1S/C26H34O4/c1-19-13-15-23(17-21(19)3)29-25(27)11-9-7-5-6-8-10-12-26(28)30
InchiKey: IRJRAYOZKLHMGA-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: Cc1ccc(OC(=O)CCCCCCCCC(=O)Oc2ccc(C)c(C)c2)cc1C
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-113.50	kJ/mol	Joback Method
hf	-642.39	kJ/mol	Joback Method
hfus	55.20	kJ/mol	Joback Method
hvap	98.98	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.552		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	3440.00		NIST Webbook
rinpol	3440.00		NIST Webbook
tb	1020.14	K	Joback Method
tc	1250.34	K	Joback Method
tf	630.02	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.56	J/mol×K	1020.14	Joback Method
cpg	1148.65	J/mol×K	1058.51	Joback Method
cpg	1161.15	J/mol×K	1096.87	Joback Method
cpg	1172.11	J/mol×K	1135.24	Joback Method
cpg	1181.56	J/mol×K	1173.61	Joback Method
cpg	1189.56	J/mol×K	1211.98	Joback Method
cpg	1196.14	J/mol×K	1250.34	Joback Method
dvisc	0.0001962	Pa×s	630.02	Joback Method

dvisc	0.0001192	Pa×s	695.04	Joback Method
dvisc	0.0000789	Pa×s	760.06	Joback Method
dvisc	0.0000557	Pa×s	825.08	Joback Method
dvisc	0.0000414	Pa×s	890.10	Joback Method
dvisc	0.0000320	Pa×s	955.12	Joback Method
dvisc	0.0000256	Pa×s	1020.14	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=U354587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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