Sebacic acid, 3,5-dimethylphenyl isobutyl ester

Inchi: InChI=1S/C22H34O4/c1-17(2)16-25-21(23)11-9-7-5-6-8-10-12-22(24)26-20-14-18(3)13-1

InchiKey: DXKXUHYOTXJIFU-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: Cc1cc(C)cc(OC(=O)CCCCCCCCC(=O)OCC(C)C)c1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-242.77	kJ/mol	Joback Method
hf	-778.70	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.529		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	891.54	K	Joback Method
tc	1096.74	K	Joback Method
tf	518.48	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.20	J/mol×K	891.54	Joback Method
cpg	1067.43	J/mol×K	1062.54	Joback Method
cpg	1055.82	J/mol×K	1028.34	Joback Method
cpg	1043.02	J/mol×K	994.14	Joback Method
cpg	1029.00	J/mol×K	959.94	Joback Method
cpg	1013.73	J/mol×K	925.74	Joback Method
cpg	1077.87	J/mol×K	1096.74	Joback Method
dvisc	0.0000384	Pa×s	891.54	Joback Method

dvisc	0.0000497	Pa×s	829.36	Joback Method
dvisc	0.0000673	Pa×s	767.19	Joback Method
dvisc	0.0000959	Pa×s	705.01	Joback Method
dvisc	0.0001465	Pa×s	642.83	Joback Method
dvisc	0.0002450	Pa×s	580.66	Joback Method
dvisc	0.0004636	Pa×s	518.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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