Sebacic acid, di(3-ethylphenyl) ester

Inchi: InChI=1S/C26H34O4/c1-3-21-13-11-15-23(19-21)29-25(27)17-9-7-5-6-8-10-18-26(28)30
InchiKey: IPGFBWALSOCWRT-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: CCc1cccc(OC(=O)CCCCCCCCC(=O)Oc2cccc(CC)c2)c1
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-94.24	kJ/mol	Joback Method
hf	-619.45	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	97.66	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.443		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	3252.00		NIST Webbook
tb	1010.18	K	Joback Method
tc	1238.38	K	Joback Method
tf	604.98	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.73	J/mol×K	1010.18	Joback Method
cpg	1151.16	J/mol×K	1048.21	Joback Method
cpg	1164.09	J/mol×K	1086.25	Joback Method
cpg	1175.57	J/mol×K	1124.28	Joback Method
cpg	1185.67	J/mol×K	1162.32	Joback Method
cpg	1194.43	J/mol×K	1200.35	Joback Method
cpg	1201.91	J/mol×K	1238.38	Joback Method
dvisc	0.0002402	Pa×s	604.98	Joback Method
dvisc	0.0001352	Pa×s	672.51	Joback Method

dvisc	0.0000846	Pa×s	740.05	Joback Method
dvisc	0.0000572	Pa×s	807.58	Joback Method
dvisc	0.0000411	Pa×s	875.11	Joback Method
dvisc	0.0000310	Pa×s	942.65	Joback Method
dvisc	0.0000242	Pa×s	1010.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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