Sebacic acid, 3,5-dimethylphenyl propyl ester

Inchi: InChI=1S/C21H32O4/c1-4-13-24-20(22)11-9-7-5-6-8-10-12-21(23)25-19-15-17(2)14-18(3
InchiKey: QZEZSYLNTIFVGK-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
hf	-878.31	kJ/mol	Cheméo Relay (1.0)
hfus	52.15	kJ/mol	Joback Method
hvap	104.13	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.77		Cheméo Relay (1.0)
logp	5.283		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2636.00		NIST Webbook
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tb	641.17	K	Cheméo Relay (1.0)
tc	844.20	K	Cheméo Relay (1.0)
tf	300.52	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	2.93100e+01
Coeff. B	1.69136e+00
Coeff. C	-8.26520e-04
Coeff. D	1.00200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.37974e+01
Coeff. B	2.99814e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	462.55
Temperature range (K), max.	720.77

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U354589&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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