Sebacic acid, 2,3-dimethylphenyl octyl ester

Inchi: InChI=1S/C26H42O4/c1-4-5-6-7-12-15-21-29-25(27)19-13-10-8-9-11-14-20-26(28)30-24
InchiKey: MWCMIKVPEBWRHR-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 418.62

Physical Properties

Property code	Value	Unit	Source
hf	-976.55	kJ/mol	Cheméo Relay (1.0)
hfus	65.10	kJ/mol	Joback Method
hvap	123.73	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.81		Cheméo Relay (1.0)
logp	7.233		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	3143.00		NIST Webbook
rinpol	3143.00		NIST Webbook
tb	674.20	K	Cheméo Relay (1.0)
tc	884.17	K	Cheméo Relay (1.0)
tf	314.14	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	2.47650e+01
Coeff. B	2.16636e+00
Coeff. C	-1.09852e-03
Coeff. D	1.59700e-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	-1.46090e+01
Coeff. B	3.46894e+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.	518.90
Temperature range (K), max.	812.10

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=U355211&Units=SI

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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