Glutaric acid, dodecyl 2-isopropylphenyl ester

Inchi: InChI=1S/C26H42O4/c1-4-5-6-7-8-9-10-11-12-15-21-29-25(27)19-16-20-26(28)30-24-18
InchiKey: JZUQMAQKZCRGFE-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 418.62

Physical Properties

Property code	Value	Unit	Source
hf	-956.39	kJ/mol	Cheméo Relay (1.0)
hfus	61.96	kJ/mol	Joback Method
hvap	120.45	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.74		Cheméo Relay (1.0)
logp	7.350		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
tb	666.10	K	Cheméo Relay (1.0)
tc	876.69	K	Cheméo Relay (1.0)
tf	300.88	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	8.78400e+00
Coeff. B	2.23176e+00
Coeff. C	-1.16876e-03
Coeff. D	1.84100e-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	-1.48370e+01
Coeff. B	3.55802e+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.	491.38
Temperature range (K), max.	807.41

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=U358857&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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