Glutaric acid, 2-methylphenyl nonyl ester

Inchi: InChI=1S/C21H32O4/c1-3-4-5-6-7-8-11-17-24-20(22)15-12-16-21(23)25-19-14-10-9-13-1
InchiKey: IRCMTMNRJVOCFC-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
af	1.0187		Cheméo Relay (1.0)
hf	-856.72	kJ/mol	Cheméo Relay (1.0)
hfus	52.54	kJ/mol	Joback Method
hvap	105.11	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-5.32		Cheméo Relay (1.0)
logp	5.365		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2616.00		NIST Webbook
tb	642.45	K	Cheméo Relay (1.0)
tc	844.58	K	Cheméo Relay (1.0)
tf	294.41	K	Cheméo Relay (1.0)
vc	1.122	m3/kmol	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	1.50110e+01
Coeff. B	1.75084e+00
Coeff. C	-8.93560e-04
Coeff. D	1.25100e-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	-1.38914e+01
Coeff. B	3.04940e+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.	450.03
Temperature range (K), max.	716.67

Sources

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=U358557&Units=SI
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

Legend

af: Acentric Factor
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
ie: Ionization energy

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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