Glutaric acid, 2-ethylphenyl tridecyl ester

Inchi: InChI=1S/C26H42O4/c1-3-5-6-7-8-9-10-11-12-13-16-22-29-25(27)20-17-21-26(28)30-24
InchiKey: WHKNFJUCNXKGBY-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1CC
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
af	1.1982		Cheméo Relay (1.0)
hf	-960.44	kJ/mol	Cheméo Relay (1.0)
hfus	65.49	kJ/mol	Joback Method
hvap	123.19	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.80		Cheméo Relay (1.0)
logp	7.179		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	673.95	K	Cheméo Relay (1.0)
tc	877.89	K	Cheméo Relay (1.0)
tf	294.26	K	Cheméo Relay (1.0)
vc	1.394	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	1.04660e+01
Coeff. B	2.22584e+00
Coeff. C	-1.16556e-03
Coeff. D	1.84600e-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	-1.47030e+01
Coeff. B	3.52020e+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.	506.38
Temperature range (K), max.	807.82

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=U358513&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
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

Latest version available from:
https://www.chemeo.com/cid/38-399-8/Glutaric-acid-2-ethylphenyl-tridecyl-ester.pdf
Generated by Cheméo on 2026-11-10 03:24:08.612820165 +0000 UTC m=+56159.541498379.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.