

Glutaric acid, 2-ethylhexyl 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C21H32O4/c1-5-7-11-18(6-2)15-24-20(22)13-9-14-21(23)25-19-12-8-10-16(3)
InchiKey:	KXOIFRUPFKMKHJ-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-251.19	kJ/mol	Joback Method
hf	-758.06	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.139		Crippen Method
mvol	297.870	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	868.66	K	Joback Method
tc	1072.18	K	Joback Method
tf	507.21	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.05	J/molxK	868.66	Joback Method
cpg	953.40	J/molxK	902.58	Joback Method
cpg	968.55	J/molxK	936.50	Joback Method
cpg	982.50	J/molxK	970.42	Joback Method
cpg	995.28	J/molxK	1004.34	Joback Method
cpg	1006.91	J/molxK	1038.26	Joback Method
cpg	1017.41	J/molxK	1072.18	Joback Method
dvisc	0.0005155	Paxs	507.21	Joback Method

dvisc	0.0002755	Paxs	567.45	Joback Method
dvisc	0.0001661	Paxs	627.69	Joback Method
dvisc	0.0001094	Paxs	687.93	Joback Method
dvisc	0.0000771	Paxs	748.18	Joback Method
dvisc	0.0000572	Paxs	808.42	Joback Method
dvisc	0.0000442	Paxs	868.66	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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