

Glutaric acid, 2-ethylhexyl isohexyl ester

Inchi:	InChI=1S/C19H36O4/c1-5-7-11-17(6-2)15-23-19(21)13-8-12-18(20)22-14-9-10-16(3)4/h1
InchiKey:	ZOLJFNPPAPLVIU-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-363.62	kJ/mol	Joback Method
hf	-935.65	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.896		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	785.82	K	Joback Method
tc	968.88	K	Joback Method
tf	418.21	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.87	J/molxK	785.82	Joback Method
cpg	927.92	J/molxK	816.33	Joback Method
cpg	944.96	J/molxK	846.84	Joback Method
cpg	961.00	J/molxK	877.35	Joback Method
cpg	976.05	J/molxK	907.86	Joback Method
cpg	990.13	J/molxK	938.37	Joback Method
cpg	1003.26	J/molxK	968.88	Joback Method
dvisc	0.0013492	Paxs	418.21	Joback Method

dvisc	0.0005543	Paxs	479.48	Joback Method
dvisc	0.0002785	Paxs	540.75	Joback Method
dvisc	0.0001610	Paxs	602.01	Joback Method
dvisc	0.0001030	Paxs	663.28	Joback Method
dvisc	0.0000711	Paxs	724.55	Joback Method
dvisc	0.0000520	Paxs	785.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
logp:	Octanol/Water partition coefficient
m_{cvol}:	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/58-634-4/Glutaric-acid-2-ethylhexyl-isoethyl-ester.pdf>

Generated by Cheméo on 2024-04-29 00:59:50.309114423 +0000 UTC m=+16641639.229691733.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.