

Glutaric acid, 2-ethylhexyl 4-chloro-2-methoxyphenyl ester

Inchi:	InChI=1S/C20H29ClO5/c1-4-6-8-15(5-2)14-25-19(22)9-7-10-20(23)26-17-12-11-16(21)1
InchiKey:	CSAKZXDXTSGMIF-UHFFFAOYSA-N
Formula:	C20H29ClO5
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	384.89

Physical Properties

Property code	Value	Unit	Source
gf	-376.54	kJ/mol	Joback Method
hf	-885.38	kJ/mol	Joback Method
hfus	48.25	kJ/mol	Joback Method
hvap	88.43	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.184		Crippen Method
mvol	301.890	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	905.63	K	Joback Method
tc	1115.10	K	Joback Method
tf	548.09	K	Joback Method
vc	1.157	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.05	J/molxK	905.63	Joback Method
cpg	947.42	J/molxK	940.54	Joback Method
cpg	960.48	J/molxK	975.45	Joback Method
cpg	972.25	J/molxK	1010.36	Joback Method
cpg	982.73	J/molxK	1045.27	Joback Method
cpg	991.93	J/molxK	1080.18	Joback Method
cpg	999.86	J/molxK	1115.10	Joback Method
dvisc	0.0003260	Paxs	548.09	Joback Method

dvisc	0.0001842	Paxs	607.68	Joback Method
dvisc	0.0001152	Paxs	667.27	Joback Method
dvisc	0.0000778	Paxs	726.86	Joback Method
dvisc	0.0000558	Paxs	786.45	Joback Method
dvisc	0.0000419	Paxs	846.04	Joback Method
dvisc	0.0000327	Paxs	905.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393910&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
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	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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