

Glutaric acid, 4-chloro-3-methylphenyl 2-octyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-4-5-6-7-9-16(3)24-19(22)10-8-11-20(23)25-17-12-13-18(21)1
InchiKey:	NPBHZE00YAKKLD-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-271.54	kJ/mol	Joback Method
hf	-753.16	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.626		Crippen Method
mvol	296.020	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	883.21	K	Joback Method
tc	1090.95	K	Joback Method
tf	525.86	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.62	J/molxK	883.21	Joback Method
cpg	967.77	J/molxK	1056.32	Joback Method
cpg	957.44	J/molxK	1021.70	Joback Method
cpg	945.98	J/molxK	987.08	Joback Method
cpg	933.37	J/molxK	952.46	Joback Method
cpg	919.59	J/molxK	917.83	Joback Method
cpg	977.00	J/molxK	1090.95	Joback Method
dvisc	0.0000439	Paxs	883.21	Joback Method

dvisc	0.0000565	Paxs	823.65	Joback Method
dvisc	0.0000755	Paxs	764.09	Joback Method
dvisc	0.0001060	Paxs	704.54	Joback Method
dvisc	0.0001586	Paxs	644.98	Joback Method
dvisc	0.0002574	Paxs	585.42	Joback Method
dvisc	0.0004662	Paxs	525.86	Joback Method

Sources

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=U391455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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