

Glutaric acid, 3-chlorophenyl 1-naphthyl ester

Inchi:	InChI=1S/C21H17ClO4/c22-16-8-4-9-17(14-16)25-20(23)12-5-13-21(24)26-19-11-3-7-15
InchiKey:	MQRSXQUBJXHQQJ-UHFFFAOYSA-N
Formula:	C21H17ClO4
SMILES:	O=C(CCCC(=O)Oc1cccc2ccccc12)Oc1ccc(Cl)c1
Mol. weight [g/mol]:	368.81

Physical Properties

Property code	Value	Unit	Source
gf	-41.62	kJ/mol	Joback Method
hf	-340.92	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.174		Crippen Method
mvol	266.890	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3137.00		NIST Webbook
rinpol	3137.00		NIST Webbook
tb	952.19	K	Joback Method
tc	1196.11	K	Joback Method
tf	611.25	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.89	J/molxK	952.19	Joback Method
cpg	790.25	J/molxK	992.84	Joback Method
cpg	800.48	J/molxK	1033.50	Joback Method
cpg	809.67	J/molxK	1074.15	Joback Method
cpg	817.88	J/molxK	1114.81	Joback Method
cpg	825.21	J/molxK	1155.46	Joback Method
cpg	831.74	J/molxK	1196.11	Joback Method
dvisc	0.0004743	Paxs	611.25	Joback Method

dvisc	0.0003184	Paxs	668.07	Joback Method
dvisc	0.0002276	Paxs	724.90	Joback Method
dvisc	0.0001708	Paxs	781.72	Joback Method
dvisc	0.0001333	Paxs	838.54	Joback Method
dvisc	0.0001073	Paxs	895.37	Joback Method
dvisc	0.0000887	Paxs	952.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390280&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

cpg:	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:	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

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