

Glutaric acid, 3-chlorophenyl (2-naphthyl)methyl ester

Inchi:	InChI=1S/C22H19ClO4/c23-19-7-3-8-20(14-19)27-22(25)10-4-9-21(24)26-15-16-11-12-1
InchiKey:	HKADCJOEKOFVBN-UHFFFAOYSA-N
Formula:	C22H19ClO4
SMILES:	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	382.84

Physical Properties

Property code	Value	Unit	Source
gf	-33.20	kJ/mol	Joback Method
hf	-361.56	kJ/mol	Joback Method
hfus	46.83	kJ/mol	Joback Method
hvap	94.78	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.312		Crippen Method
mvol	280.980	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	975.07	K	Joback Method
tc	1217.08	K	Joback Method
tf	622.52	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.46	J/molxK	975.07	Joback Method
cpg	883.67	J/molxK	1176.74	Joback Method
cpg	876.14	J/molxK	1136.41	Joback Method
cpg	867.74	J/molxK	1096.07	Joback Method
cpg	858.39	J/molxK	1055.74	Joback Method
cpg	847.99	J/molxK	1015.40	Joback Method
cpg	890.40	J/molxK	1217.08	Joback Method
dvisc	0.0000774	Paxs	975.07	Joback Method

dvisc	0.0000940	Paxs	916.31	Joback Method
dvisc	0.0001173	Paxs	857.55	Joback Method
dvisc	0.0001512	Paxs	798.79	Joback Method
dvisc	0.0002028	Paxs	740.04	Joback Method
dvisc	0.0002863	Paxs	681.28	Joback Method
dvisc	0.0004312	Paxs	622.52	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=U392206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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