

Glutaric acid, 2,3-dichlorophenyl 1-naphthyl ester

Inchi:	InChI=1S/C21H16Cl2O4/c22-16-9-4-11-18(21(16)23)27-20(25)13-5-12-19(24)26-17-10-3
InchiKey:	KLEGTRFNGPZTEH-UHFFFAOYSA-N
Formula:	C21H16Cl2O4
SMILES:	O=C(CCCC(=O)Oc1cccc2ccccc12)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	403.25

Physical Properties

Property code	Value	Unit	Source
gf	-63.18	kJ/mol	Joback Method
hf	-368.13	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	97.60	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.828		Crippen Method
mvol	279.130	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	994.60	K	Joback Method
tc	1242.36	K	Joback Method
tf	653.69	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.99	J/molxK	994.60	Joback Method
cpg	836.11	J/molxK	1201.06	Joback Method
cpg	829.94	J/molxK	1159.77	Joback Method
cpg	822.92	J/molxK	1118.48	Joback Method
cpg	814.98	J/molxK	1077.19	Joback Method
cpg	806.03	J/molxK	1035.89	Joback Method
cpg	841.50	J/molxK	1242.36	Joback Method
dvisc	0.0000788	Paxs	994.60	Joback Method

dvisc	0.0000945	Paxs	937.78	Joback Method
dvisc	0.0001160	Paxs	880.96	Joback Method
dvisc	0.0001465	Paxs	824.14	Joback Method
dvisc	0.0001915	Paxs	767.33	Joback Method
dvisc	0.0002613	Paxs	710.51	Joback Method
dvisc	0.0003764	Paxs	653.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393261&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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