Glutaric acid, naphth-2-ylmethyl 2,4-dichlorophenyl ester

Inchi: InChI=1S/C22H18Cl2O4/c23-18-10-11-20(19(24)13-18)28-22(26)7-3-6-21(25)27-14-15-8

InchiKey: JDSSBLJUTLYLHO-UHFFFAOYSA-N

Formula: C22H18Cl2O4

SMILES: O=C(CCCC(=O)Oc1ccc(Cl)cc1Cl)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 417.28

Physical Properties

Property code	Value	Unit	Source
gf	-54.76	kJ/mol	Joback Method
hf	-388.77	kJ/mol	Joback Method
hfus	50.64	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	5.966		Crippen Method
mcvol	293.220	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	3416.00		NIST Webbook
rinpol	3416.00		NIST Webbook
tb	1017.48	K	Joback Method
tc	1263.90	K	Joback Method
tf	664.96	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.66	J/mol×K	1017.48	Joback Method
cpg	894.71	J/mol×K	1222.83	Joback Method
cpg	888.35	J/mol×K	1181.76	Joback Method
cpg	881.14	J/mol×K	1140.69	Joback Method
cpg	873.01	J/mol×K	1099.62	Joback Method
cpg	863.88	J/mol×K	1058.55	Joback Method
cpg	900.32	J/mol×K	1263.90	Joback Method
dvisc	0.0000685	Pa×s	1017.48	Joback Method

dvisc	0.0000825	Pa×s	958.73	Joback Method
dvisc	0.0001017	Pa×s	899.97	Joback Method
dvisc	0.0001291	Pa×s	841.22	Joback Method
dvisc	0.0001699	Pa×s	782.47	Joback Method
dvisc	0.0002338	Pa×s	723.71	Joback Method
dvisc	0.0003404	Pa×s	664.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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