Glutaric acid, naphth-2-ylmethyl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C23H21ClO4/c1-16-9-12-20(24)21(13-16)28-23(26)8-4-7-22(25)27-15-17-10-1

InchiKey: RYMIZFMTZULDMM-UHFFFAOYSA-N

Formula: C23H21ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCC(=O)OCc2ccc3ccccc3c2)c1

Mol. weight [g/mol]: 396.86

Physical Properties

Property code	Value	Unit	Source
gf	-34.41	kJ/mol	Joback Method
hf	-393.67	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	97.67	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.621		Crippen Method
mcvol	295.070	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	3352.00		NIST Webbook
rinpol	3352.00		NIST Webbook
tb	1002.93	K	Joback Method
tc	1244.64	K	Joback Method
tf	646.31	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.16	J/mol×K	1002.93	Joback Method
cpg	904.72	J/mol×K	1043.21	Joback Method
cpg	915.11	J/mol×K	1083.50	Joback Method
cpg	924.43	J/mol×K	1123.78	Joback Method
cpg	932.75	J/mol×K	1164.07	Joback Method
cpg	940.15	J/mol×K	1204.35	Joback Method
cpg	946.70	J/mol×K	1244.64	Joback Method
dvisc	0.0003611	Pa×s	646.31	Joback Method

dvisc	0.0002443	Pa×s	705.75	Joback Method
dvisc	0.0001756	Pa×s	765.18	Joback Method
dvisc	0.0001324	Pa×s	824.62	Joback Method
dvisc	0.0001036	Pa×s	884.06	Joback Method
dvisc	0.0000837	Pa×s	943.49	Joback Method
dvisc	0.0000693	Pa×s	1002.93	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=U393434&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