

Glutaric acid, naphth-2-ylmethyl 2-methyl-4-chlorophenyl ester

Inchi:	InChI=1S/C23H21ClO4/c1-16-13-20(24)11-12-21(16)28-23(26)8-4-7-22(25)27-15-17-9-1
InchiKey:	KZONOCKYRQJVHR-UHFFFAOYSA-N
Formula:	C23H21ClO4
SMILES:	<chem>Cc1cc(Cl)ccc1OC(=O)CCCC(=O)OCc1ccc2ccccc2c1</chem>
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	3373.00		NIST Webbook
rinpol	3373.00		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/molxK	1002.93	Joback Method
cpg	940.15	J/molxK	1204.35	Joback Method
cpg	932.75	J/molxK	1164.07	Joback Method
cpg	924.43	J/molxK	1123.78	Joback Method
cpg	915.11	J/molxK	1083.50	Joback Method
cpg	904.72	J/molxK	1043.21	Joback Method
cpg	946.70	J/molxK	1244.64	Joback Method
dvisc	0.0000693	Paxs	1002.93	Joback Method

dvisc	0.0000837	Paxs	943.49	Joback Method
dvisc	0.0001036	Paxs	884.06	Joback Method
dvisc	0.0001324	Paxs	824.62	Joback Method
dvisc	0.0001756	Paxs	765.18	Joback Method
dvisc	0.0002443	Paxs	705.75	Joback Method
dvisc	0.0003611	Paxs	646.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392082&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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