

Succinic acid, naphth-2-ylmethyl 2-chloro-4-methylphenyl ester

Inchi:	InChI=1S/C22H19ClO4/c1-15-6-9-20(19(23)12-15)27-22(25)11-10-21(24)26-14-16-7-8-1
InchiKey:	DENJQCLUBGHGJC-UHFFFAOYSA-N
Formula:	C22H19ClO4
SMILES:	<chem>Cc1ccc(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)c(Cl)c1</chem>
Mol. weight [g/mol]:	382.84

Physical Properties

Property code	Value	Unit	Source
gf	-42.83	kJ/mol	Joback Method
hf	-373.03	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	95.44	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.231		Crippen Method
mvol	280.980	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	3299.00		NIST Webbook
rinpol	3299.00		NIST Webbook
tb	980.05	K	Joback Method
tc	1222.80	K	Joback Method
tf	635.04	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.91	J/molxK	980.05	Joback Method
cpg	881.18	J/molxK	1182.34	Joback Method
cpg	873.93	J/molxK	1141.88	Joback Method
cpg	865.76	J/molxK	1101.43	Joback Method
cpg	856.58	J/molxK	1060.97	Joback Method
cpg	846.32	J/molxK	1020.51	Joback Method
cpg	887.58	J/molxK	1222.80	Joback Method
dvisc	0.0000795	Paxs	980.05	Joback Method

dvisc	0.0000956	Paxs	922.55	Joback Method
dvisc	0.0001179	Paxs	865.05	Joback Method
dvisc	0.0001497	Paxs	807.54	Joback Method
dvisc	0.0001973	Paxs	750.04	Joback Method
dvisc	0.0002721	Paxs	692.54	Joback Method
dvisc	0.0003979	Paxs	635.04	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=U390225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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