Succinic acid, naphth-2-ylmethyl 3-chlorophenyl ester

Inchi: InChI=1S/C21H17ClO4/c22-18-6-3-7-19(13-18)26-21(24)11-10-20(23)25-14-15-8-9-16-4

InchiKey: FCOQAFJOMJBLAO-UHFFFAOYSA-N

Formula: C21H17ClO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 368.81

Physical Properties

Property code	Value	Unit	Source
gf	-41.62	kJ/mol	Joback Method
hf	-340.92	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.922		Crippen Method
mcvol	266.890	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	952.19	K	Joback Method
tc	1196.11	K	Joback Method
tf	611.25	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.89	J/mol×K	952.19	Joback Method
cpg	790.25	J/mol×K	992.84	Joback Method
cpg	800.48	J/mol×K	1033.50	Joback Method
cpg	809.67	J/mol×K	1074.15	Joback Method
cpg	817.88	J/mol×K	1114.81	Joback Method
cpg	825.21	J/mol×K	1155.46	Joback Method
cpg	831.74	J/mol×K	1196.11	Joback Method
dvisc	0.0004743	Pa×s	611.25	Joback Method

dvisc	0.0003184	Pa×s	668.07	Joback Method
dvisc	0.0002276	Pa×s	724.90	Joback Method
dvisc	0.0001708	Pa×s	781.72	Joback Method
dvisc	0.0001333	Pa×s	838.54	Joback Method
dvisc	0.0001073	Pa×s	895.37	Joback Method
dvisc	0.0000887	Pa×s	952.19	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=U389861&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