

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

Inchi:	InChI=1S/C22H19ClO5/c1-26-20-13-18(23)8-9-19(20)28-22(25)11-10-21(24)27-14-15-6
InchiKey:	GFIMVROKICWILT-UHFFFAOYSA-N
Formula:	C22H19ClO5
SMILES:	COc1cc(Cl)ccc1OC(=O)CCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	398.84

Physical Properties

Property code	Value	Unit	Source
gf	-147.83	kJ/mol	Joback Method
hf	-505.25	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	97.85	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.931		Crippen Method
mvol	286.850	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1002.47	K	Joback Method
tc	1244.75	K	Joback Method
tf	657.27	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.86	J/molxK	1002.47	Joback Method
cpg	899.42	J/molxK	1204.37	Joback Method
cpg	893.91	J/molxK	1163.99	Joback Method
cpg	887.25	J/molxK	1123.61	Joback Method
cpg	879.39	J/molxK	1083.23	Joback Method
cpg	870.28	J/molxK	1042.85	Joback Method
cpg	903.84	J/molxK	1244.75	Joback Method
dvisc	0.0000595	Paxs	1002.47	Joback Method

dvisc	0.0000715	Paxs	944.94	Joback Method
dvisc	0.0000880	Paxs	887.40	Joback Method
dvisc	0.0001115	Paxs	829.87	Joback Method
dvisc	0.0001463	Paxs	772.34	Joback Method
dvisc	0.0002006	Paxs	714.80	Joback Method
dvisc	0.0002907	Paxs	657.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390948&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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