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

Inchi: InChI=1S/C23H22O4/c1-2-17-6-5-9-21(15-17)27-23(25)13-12-22(24)26-16-18-10-11-19-
InchiKey: XMOWUHBTKFCDGK-UHFFFAOYSA-N
Formula: C23H22O4
SMILES: CCc1cccc(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)c1
Mol. weight [g/mol]: 362.42

Physical Properties

Property code	Value	Unit	Source
gf	-12.85	kJ/mol	Joback Method
hf	-366.46	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	92.62	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.831		Crippen Method
mcvol	282.830	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	3077.00		NIST Webbook
rinpol	3077.00		NIST Webbook
tb	960.52	K	Joback Method
tc	1197.59	K	Joback Method
tf	603.87	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.15	J/mol×K	960.52	Joback Method
cpg	887.05	J/mol×K	1000.03	Joback Method
cpg	898.77	J/mol×K	1039.54	Joback Method
cpg	909.37	J/mol×K	1079.06	Joback Method
cpg	918.94	J/mol×K	1118.57	Joback Method
cpg	927.56	J/mol×K	1158.08	Joback Method
cpg	935.31	J/mol×K	1197.59	Joback Method
dvisc	0.0004574	Pa×s	603.87	Joback Method

dvisc	0.0002984	Pa×s	663.31	Joback Method
dvisc	0.0002088	Pa×s	722.75	Joback Method
dvisc	0.0001542	Pa×s	782.19	Joback Method
dvisc	0.0001189	Pa×s	841.64	Joback Method
dvisc	0.0000949	Pa×s	901.08	Joback Method
dvisc	0.0000779	Pa×s	960.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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