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

Inchi: InChI=1S/C21H15ClO4/c22-18-6-3-7-19(13-18)26-21(24)11-10-20(23)25-14-15-8-9-16-4

InchiKey: JOJMNJMYFPMZSC-ZHACJKMWSA-N

Formula: C21H15ClO4

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

Mol. weight [g/mol]: 366.79

Physical Properties

Property code	Value	Unit	Source
gf	38.60	kJ/mol	Joback Method
hf	-223.70	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.698		Crippen Method
mcvol	262.590	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	956.35	K	Joback Method
tc	1206.80	K	Joback Method
tf	606.17	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.87	J/mol×K	956.35	Joback Method
cpg	797.15	J/mol×K	1165.06	Joback Method
cpg	789.22	J/mol×K	1123.31	Joback Method
cpg	780.63	J/mol×K	1081.57	Joback Method
cpg	771.28	J/mol×K	1039.83	Joback Method
cpg	761.06	J/mol×K	998.09	Joback Method
cpg	804.54	J/mol×K	1206.80	Joback Method
dvisc	0.0000779	Pa×s	956.35	Joback Method

dvisc	0.0000945	Pa×s	897.99	Joback Method
dvisc	0.0001177	Pa×s	839.62	Joback Method
dvisc	0.0001515	Pa×s	781.26	Joback Method
dvisc	0.0002032	Pa×s	722.90	Joback Method
dvisc	0.0002869	Pa×s	664.53	Joback Method
dvisc	0.0004328	Pa×s	606.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405857&Units=SI

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