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

Inchi: InChI=1S/C20H13ClO4/c21-16-6-3-7-17(13-16)24-19(22)10-11-20(23)25-18-9-8-14-4-1-2
InchiKey: HGLSZGDWKLONDY-ZHACJKMWSA-N
Formula: C20H13ClO4
SMILES: O=C(C=CC(=O)Oc1ccc2ccccc2c1)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 352.77

Physical Properties

Property code	Value	Unit	Source
gf	30.18	kJ/mol	Joback Method
hf	-203.06	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.560		Crippen Method
mcvol	248.500	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	2965.00		NIST Webbook
rinpol	2965.00		NIST Webbook
tb	933.47	K	Joback Method
tc	1187.29	K	Joback Method
tf	594.90	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.23	J/mol×K	933.47	Joback Method
cpg	739.00	J/mol×K	1144.99	Joback Method
cpg	731.40	J/mol×K	1102.69	Joback Method
cpg	723.14	J/mol×K	1060.38	Joback Method
cpg	714.09	J/mol×K	1018.08	Joback Method
cpg	704.16	J/mol×K	975.77	Joback Method
cpg	746.04	J/mol×K	1187.29	Joback Method
dvisc	0.0000889	Pa×s	933.47	Joback Method

dvisc	0.0001074	Pa×s	877.04	Joback Method
dvisc	0.0001332	Pa×s	820.61	Joback Method
dvisc	0.0001705	Pa×s	764.19	Joback Method
dvisc	0.0002270	Pa×s	707.76	Joback Method
dvisc	0.0003177	Pa×s	651.33	Joback Method
dvisc	0.0004738	Pa×s	594.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405832&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