Fumaric acid, 2,4,6-trichlorophenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H13Cl3O4/c22-16-10-17(23)21(18(24)11-16)28-20(26)8-7-19(25)27-12-13-

InchiKey: XBXWHVZVHWETCP-BQYQJAHWSA-N

Formula: C21H13Cl3O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 435.69

Physical Properties

Property code	Value	Unit	Source
gf	-4.52	kJ/mol	Joback Method
hf	-278.12	kJ/mol	Joback Method
hfus	52.06	kJ/mol	Joback Method
hvap	102.60	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.005		Crippen Method
mcvol	287.070	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	3227.00		NIST Webbook
tb	1041.17	K	Joback Method
tc	1298.66	K	Joback Method
tf	691.05	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.46	J/mol×K	1041.17	Joback Method
cpg	818.82	J/mol×K	1255.74	Joback Method
cpg	812.60	J/mol×K	1212.83	Joback Method
cpg	805.86	J/mol×K	1169.91	Joback Method
cpg	798.49	J/mol×K	1127.00	Joback Method
cpg	790.39	J/mol×K	1084.08	Joback Method
cpg	824.62	J/mol×K	1298.66	Joback Method
dvisc	0.0000613	Pa×s	1041.17	Joback Method
dvisc	0.0000731	Pa×s	982.82	Joback Method

dvisc	0.0000891	Pa×s	924.46	Joback Method
dvisc	0.0001115	Pa×s	866.11	Joback Method
dvisc	0.0001442	Pa×s	807.76	Joback Method
dvisc	0.0001940	Pa×s	749.40	Joback Method
dvisc	0.0002744	Pa×s	691.05	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=U405960&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