Fumaric acid, 2,6-dichlorophenyl 2-ethylhexyl ester

Inchi: InChI=1S/C18H22Cl2O4/c1-3-5-7-13(4-2)12-23-16(21)10-11-17(22)24-18-14(19)8-6-9-15

InchiKey: IXVYZOIIOCRRTA-ZHACJKMWSA-N

Formula: C18H22Cl2O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-220.09	kJ/mol	Joback Method
hf	-610.40	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.215		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	879.04	K	Joback Method
tc	1095.34	K	Joback Method
tf	528.16	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.49	J/mol×K	879.04	Joback Method
cpg	798.45	J/mol×K	915.09	Joback Method
cpg	810.36	J/mol×K	951.14	Joback Method
cpg	821.26	J/mol×K	987.19	Joback Method
cpg	831.18	J/mol×K	1023.24	Joback Method
cpg	840.15	J/mol×K	1059.29	Joback Method
cpg	848.20	J/mol×K	1095.34	Joback Method
dvisc	0.0004334	Pa×s	528.16	Joback Method

dvisc	0.0002447	Pa×s	586.64	Joback Method
dvisc	0.0001532	Pa×s	645.12	Joback Method
dvisc	0.0001037	Pa×s	703.60	Joback Method
dvisc	0.0000745	Pa×s	762.08	Joback Method
dvisc	0.0000561	Pa×s	820.56	Joback Method
dvisc	0.0000439	Pa×s	879.04	Joback Method

Sources

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=U405863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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