Fumaric acid, 2,4-dichlorophenyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H14Cl2O4/c1-3-5-12(4-2)21-15(19)8-9-16(20)22-14-7-6-11(17)10-13(14)18

InchiKey: MFZOERMALNZLAH-CMDGGOBGSA-N

Formula: C16H14Cl2O4

SMILES: CC#CC(CC)OC(=O)C=CC(=O)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 341.19

Physical Properties

Property code	Value	Unit	Source
gf	-34.13	kJ/mol	Joback Method
hf	-296.82	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	83.61	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.800		Crippen Method
mcvol	239.000	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	842.28	K	Joback Method
tc	1079.45	K	Joback Method
tf	611.72	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.10	J/mol×K	842.28	Joback Method
cpg	631.77	J/mol×K	881.81	Joback Method
cpg	642.41	J/mol×K	921.34	Joback Method
cpg	652.03	J/mol×K	960.86	Joback Method
cpg	660.67	J/mol×K	1000.39	Joback Method
cpg	668.35	J/mol×K	1039.92	Joback Method
cpg	675.10	J/mol×K	1079.45	Joback Method

Sources

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=U405696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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