Fumaric acid, 2,4,6-trichlorophenyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H13Cl3O4/c1-3-5-11(4-2)22-14(20)6-7-15(21)23-16-12(18)8-10(17)9-13(16

InchiKey: IRZKPHVZWFPEKE-VOTSOKGWSA-N

Formula: C16H13Cl3O4

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

Mol. weight [g/mol]: 375.63

Physical Properties

Property code	Value	Unit	Source
gf	-55.69	kJ/mol	Joback Method
hf	-324.03	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.454		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	884.69	K	Joback Method
tc	1125.05	K	Joback Method
tf	654.16	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.64	J/mol×K	884.69	Joback Method
cpg	649.05	J/mol×K	924.75	Joback Method
cpg	658.42	J/mol×K	964.81	Joback Method
cpg	666.79	J/mol×K	1004.87	Joback Method
cpg	674.17	J/mol×K	1044.93	Joback Method
cpg	680.58	J/mol×K	1084.99	Joback Method
cpg	686.06	J/mol×K	1125.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405953&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

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