Fumaric acid, hexadecyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C26H37Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-32-24(30)16-17-25(31

InchiKey: OERIBWCXCWLROJ-WUKNDPDISA-N

Formula: C26H37Cl3O4

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

Mol. weight [g/mol]: 519.93

Physical Properties

Property code	Value	Unit	Source
gf	-171.85	kJ/mol	Joback Method
hf	-797.45	kJ/mol	Joback Method
hfus	74.34	kJ/mol	Joback Method
hvap	109.16	kJ/mol	Joback Method
log10ws	-10.09		Crippen Method
logp	9.133		Crippen Method
mcvol	400.740	ml/mol	McGowan Method
pc	867.60	kPa	Joback Method
rinpol	3547.00		NIST Webbook
tb	1104.93	K	Joback Method
tc	1357.88	K	Joback Method
tf	675.76	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.94	J/mol×K	1104.93	Joback Method
cpg	1297.75	J/mol×K	1147.09	Joback Method
cpg	1310.03	J/mol×K	1189.25	Joback Method
cpg	1320.85	J/mol×K	1231.41	Joback Method
cpg	1330.31	J/mol×K	1273.57	Joback Method
cpg	1338.49	J/mol×K	1315.72	Joback Method
cpg	1345.49	J/mol×K	1357.88	Joback Method
dvisc	0.0001131	Pa×s	675.76	Joback Method
dvisc	0.0000654	Pa×s	747.29	Joback Method

dvisc	0.0000417	Pa×s	818.82	Joback Method
dvisc	0.0000285	Pa×s	890.34	Joback Method
dvisc	0.0000206	Pa×s	961.87	Joback Method
dvisc	0.0000156	Pa×s	1033.40	Joback Method
dvisc	0.0000123	Pa×s	1104.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348279&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