Fumaric acid, 2,5-dichlorophenyl hept-2-yl ester

Inchi: InChI=1S/C17H20Cl2O4/c1-3-4-5-6-12(2)22-16(20)9-10-17(21)23-15-11-13(18)7-8-14(15

InchiKey: ARMCTUPTAACPSR-MDZDMXLPSA-N

Formula: C17H20Cl2O4

SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 359.24

Physical Properties

Property code	Value	Unit	Source
gf	-228.51	kJ/mol	Joback Method
hf	-589.76	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	83.69	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.967		Crippen Method
mcvol	261.690	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	856.16	K	Joback Method
tc	1073.35	K	Joback Method
tf	516.89	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.69	J/mol×K	856.16	Joback Method
cpg	741.40	J/mol×K	892.36	Joback Method
cpg	753.09	J/mol×K	928.56	Joback Method
cpg	763.80	J/mol×K	964.76	Joback Method
cpg	773.55	J/mol×K	1000.95	Joback Method
cpg	782.37	J/mol×K	1037.15	Joback Method
cpg	790.29	J/mol×K	1073.35	Joback Method
dvisc	0.0004807	Pa×s	516.89	Joback Method

dvisc	0.0002746	Pa×s	573.43	Joback Method
dvisc	0.0001735	Pa×s	629.98	Joback Method
dvisc	0.0001182	Pa×s	686.52	Joback Method
dvisc	0.0000854	Pa×s	743.07	Joback Method
dvisc	0.0000646	Pa×s	799.61	Joback Method
dvisc	0.0000507	Pa×s	856.16	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=U405969&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