

Fumaric acid, 2,6-dichlorophenyl hept-2-yl ester

Inchi:	InChI=1S/C17H20Cl2O4/c1-3-4-5-7-12(2)22-15(20)10-11-16(21)23-17-13(18)8-6-9-14(19)
InchiKey:	QYMWSNKZHALFEA-ZHACJKMWSA-N
Formula:	C17H20Cl2O4
SMILES:	CCCCC(C)OC(=O)C=CC(=O)Oc1c(Cl)cccc1Cl
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
mvol	261.690	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2358.00		NIST Webbook
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tb	856.16	K	Joback Method
tc	1073.35	K	Joback Method
tf	516.89	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002746	Paxs	573.43	Joback Method
dvisc	0.0001735	Paxs	629.98	Joback Method
dvisc	0.0001182	Paxs	686.52	Joback Method
dvisc	0.0000854	Paxs	743.07	Joback Method
dvisc	0.0000646	Paxs	799.61	Joback Method
dvisc	0.0000507	Paxs	856.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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