

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

Inchi:	InChI=1S/C15H15Cl3O4/c1-2-3-4-7-21-13(19)5-6-14(20)22-15-11(17)8-10(16)9-12(15)18
InchiKey:	KQBJGULELVKICC-AATRIKPKSA-N
Formula:	C15H15Cl3O4
SMILES:	CCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	365.64

Physical Properties

Property code	Value	Unit	Source
gf	-264.47	kJ/mol	Joback Method
hf	-570.41	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.842		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2383.00		NIST Webbook
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tb	853.25	K	Joback Method
tc	1075.15	K	Joback Method
tf	551.79	K	Joback Method
vc	0.943	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.32	J/molxK	853.25	Joback Method
cpg	648.11	J/molxK	890.23	Joback Method
cpg	657.98	J/molxK	927.22	Joback Method
cpg	666.96	J/molxK	964.20	Joback Method
cpg	675.06	J/molxK	1001.18	Joback Method
cpg	682.30	J/molxK	1038.17	Joback Method
cpg	688.71	J/molxK	1075.15	Joback Method
dvisc	0.0003929	Paxs	551.79	Joback Method

dvisc	0.0002561	Paxs	602.03	Joback Method
dvisc	0.0001783	Paxs	652.28	Joback Method
dvisc	0.0001308	Paxs	702.52	Joback Method
dvisc	0.0000999	Paxs	752.76	Joback Method
dvisc	0.0000790	Paxs	803.01	Joback Method
dvisc	0.0000642	Paxs	853.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348271&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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