

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

Inchi:	InChI=1S/C20H26Cl2O4/c1-3-4-5-6-7-8-9-15(2)25-19(23)12-13-20(24)26-18-14-16(21)10
InchiKey:	UNIWKHSLIJBAAZ-OUKQBFOZSA-N
Formula:	C20H26Cl2O4
SMILES:	CCCCCCCCC(C)OC(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	401.32

Physical Properties

Property code	Value	Unit	Source
gf	-203.25	kJ/mol	Joback Method
hf	-651.68	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	90.37	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.137		Crippen Method
mcvol	303.960	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2690.00		NIST Webbook
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tb	924.80	K	Joback Method
tc	1141.54	K	Joback Method
tf	550.70	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.42	J/molxK	924.80	Joback Method
cpg	957.70	J/molxK	1105.42	Joback Method
cpg	948.52	J/molxK	1069.30	Joback Method
cpg	938.34	J/molxK	1033.17	Joback Method
cpg	927.12	J/molxK	997.05	Joback Method
cpg	914.83	J/molxK	960.92	Joback Method
cpg	965.93	J/molxK	1141.54	Joback Method
dvisc	0.0000328	Paxs	924.80	Joback Method

dvisc	0.0000422	Paxs	862.45	Joback Method
dvisc	0.0000564	Paxs	800.10	Joback Method
dvisc	0.0000792	Paxs	737.75	Joback Method
dvisc	0.0001185	Paxs	675.40	Joback Method
dvisc	0.0001923	Paxs	613.05	Joback Method
dvisc	0.0003484	Paxs	550.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405973&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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