

Fumaric acid, 4-octyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H22Cl2O4/c1-3-5-8-13(7-4-2)23-16(21)11-12-17(22)24-15-10-6-9-14(19)18
InchiKey: RKBYZZLQSHUYMJ-VAWYXSNFSA-N
Formula: C18H22Cl2O4
SMILES: CCCCC(CCC)OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-220.09	kJ/mol	Joback Method
hf	-610.40	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.357		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2487.00		NIST Webbook
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tb	879.04	K	Joback Method
tc	1095.34	K	Joback Method
tf	528.16	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.49	J/molxK	879.04	Joback Method
cpg	798.45	J/molxK	915.09	Joback Method
cpg	810.36	J/molxK	951.14	Joback Method
cpg	821.26	J/molxK	987.19	Joback Method
cpg	831.18	J/molxK	1023.24	Joback Method
cpg	840.15	J/molxK	1059.29	Joback Method
cpg	848.20	J/molxK	1095.34	Joback Method
dvisc	0.0004334	Paxs	528.16	Joback Method

dvisc	0.0002447	Paxs	586.64	Joback Method
dvisc	0.0001532	Paxs	645.12	Joback Method
dvisc	0.0001037	Paxs	703.60	Joback Method
dvisc	0.0000745	Paxs	762.08	Joback Method
dvisc	0.0000561	Paxs	820.56	Joback Method
dvisc	0.0000439	Paxs	879.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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