Fumaric acid, 3,5-dichlorophenyl pentyl ester

Inchi: InChI=1S/C15H16Cl2O4/c1-2-3-4-7-20-14(18)5-6-15(19)21-13-9-11(16)8-12(17)10-13/h5
InchiKey: RXVXYTPKGNCKMZ-AATRIKPKSA-N
Formula: C15H16Cl2O4
SMILES: CCCCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-242.91	kJ/mol	Joback Method
hf	-543.20	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.188		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	810.84	K	Joback Method
tc	1028.62	K	Joback Method
tf	509.35	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.15	J/mol×K	810.84	Joback Method
cpg	629.09	J/mol×K	847.14	Joback Method
cpg	640.12	J/mol×K	883.43	Joback Method
cpg	650.25	J/mol×K	919.73	Joback Method
cpg	659.51	J/mol×K	956.03	Joback Method
cpg	667.91	J/mol×K	992.32	Joback Method
cpg	675.49	J/mol×K	1028.62	Joback Method
dvisc	0.0005264	Pa×s	509.35	Joback Method

dvisc	0.0003265	Pa×s	559.60	Joback Method
dvisc	0.0002191	Pa×s	609.85	Joback Method
dvisc	0.0001562	Pa×s	660.10	Joback Method
dvisc	0.0001169	Pa×s	710.34	Joback Method
dvisc	0.0000908	Pa×s	760.59	Joback Method
dvisc	0.0000729	Pa×s	810.84	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=U348235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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