Fumaric acid, di(8-chlorooctyl) ester

Inchi: InChI=1S/C20H34Cl2O4/c21-15-9-5-1-3-7-11-17-25-19(23)13-14-20(24)26-18-12-8-4-2-6
InchiKey: QMQZGFHUZRFAIY-BUHFOSPRSA-N
Formula: C20H34Cl2O4
SMILES: O=C(C=CC(=O)OCCCCCCCCCCl)OCCCCCCCCCCl
Mol. weight [g/mol]: 409.39

Physical Properties

Property code	Value	Unit	Source
gf	-293.96	kJ/mol	Joback Method
hf	-859.99	kJ/mol	Joback Method
hfus	61.73	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.788		Crippen Method
mcvol	327.720	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	888.60	K	Joback Method
tc	1088.64	K	Joback Method
tf	514.24	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.09	J/mol×K	888.60	Joback Method
cpg	1018.99	J/mol×K	921.94	Joback Method
cpg	1033.83	J/mol×K	955.28	Joback Method
cpg	1047.65	J/mol×K	988.62	Joback Method
cpg	1060.50	J/mol×K	1021.96	Joback Method
cpg	1072.40	J/mol×K	1055.30	Joback Method
cpg	1083.39	J/mol×K	1088.64	Joback Method
dvisc	0.0004822	Pa×s	514.24	Joback Method

dvisc	0.0002434	Pa×s	576.63	Joback Method
dvisc	0.0001404	Pa×s	639.03	Joback Method
dvisc	0.0000893	Pa×s	701.42	Joback Method
dvisc	0.0000612	Pa×s	763.81	Joback Method
dvisc	0.0000444	Pa×s	826.21	Joback Method
dvisc	0.0000337	Pa×s	888.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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