Fumaric acid, di(10-chlorodecyl) ester

Inchi: InChI=1S/C24H42Cl2O4/c25-19-13-9-5-1-3-7-11-15-21-29-23(27)17-18-24(28)30-22-16-
InchiKey: QQCGGPBFZAAEAI-ISLYRVAYSA-N
Formula: C24H42Cl2O4
SMILES: O=C(C=CC(=O)OCCCCCCCCCCCCl)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 465.49

Physical Properties

Property code	Value	Unit	Source
gf	-260.28	kJ/mol	Joback Method
hf	-942.55	kJ/mol	Joback Method
hfus	72.09	kJ/mol	Joback Method
hvap	96.06	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.348		Crippen Method
mcvol	384.080	ml/mol	McGowan Method
pc	839.19	kPa	Joback Method
rinpol	3469.00		NIST Webbook
rinpol	3469.00		NIST Webbook
tb	980.12	K	Joback Method
tc	1203.91	K	Joback Method
tf	559.32	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.82	J/mol×K	980.12	Joback Method
cpg	1266.67	J/mol×K	1017.42	Joback Method
cpg	1283.14	J/mol×K	1054.72	Joback Method
cpg	1298.28	J/mol×K	1092.02	Joback Method
cpg	1312.16	J/mol×K	1129.31	Joback Method
cpg	1324.85	J/mol×K	1166.61	Joback Method
cpg	1336.42	J/mol×K	1203.91	Joback Method
dvisc	0.0002915	Pa×s	559.32	Joback Method

dvisc	0.0001416	Pa×s	629.45	Joback Method
dvisc	0.0000795	Pa×s	699.59	Joback Method
dvisc	0.0000496	Pa×s	769.72	Joback Method
dvisc	0.0000334	Pa×s	839.85	Joback Method
dvisc	0.0000240	Pa×s	909.99	Joback Method
dvisc	0.0000180	Pa×s	980.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348315&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