Fumaric acid, 2-chloropropyl tridecyl ester

Inchi: InChI=1S/C20H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-16-24-19(22)14-15-20(23)25-17-18
InchiKey: QLRKWJUGPGGUET-CCEZHUSRSA-N
Formula: C20H35ClO4
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 374.94

Physical Properties

Property code	Value	Unit	Source
gf	-284.47	kJ/mol	Joback Method
hf	-849.53	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.567		Crippen Method
mcvol	315.480	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	850.73	K	Joback Method
tc	1044.27	K	Joback Method
tf	469.32	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.00	J/mol×K	850.73	Joback Method
cpg	1049.09	J/mol×K	1012.02	Joback Method
cpg	1036.24	J/mol×K	979.76	Joback Method
cpg	1022.43	J/mol×K	947.50	Joback Method
cpg	1007.65	J/mol×K	915.24	Joback Method
cpg	991.85	J/mol×K	882.99	Joback Method
cpg	1061.03	J/mol×K	1044.27	Joback Method
dvisc	0.0000364	Pa×s	850.73	Joback Method
dvisc	0.0000489	Pa×s	787.16	Joback Method

dvisc	0.0000693	Pa×s	723.59	Joback Method
dvisc	0.0001049	Pa×s	660.02	Joback Method
dvisc	0.0001734	Pa×s	596.46	Joback Method
dvisc	0.0003234	Pa×s	532.89	Joback Method
dvisc	0.0007139	Pa×s	469.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348571&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

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