Fumaric acid, 10-chlorodecyl decyl ester

Inchi: InChI=1S/C24H43ClO4/c1-2-3-4-5-6-10-13-16-21-28-23(26)18-19-24(27)29-22-17-14-11
InchiKey: LOOMFFOETFJREH-VHEBQXMUSA-N
Formula: C24H43ClO4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCCCl
Mol. weight [g/mol]: 431.05

Physical Properties

Property code	Value	Unit	Source
gf	-248.35	kJ/mol	Joback Method
hf	-926.81	kJ/mol	Joback Method
hfus	67.89	kJ/mol	Joback Method
hvap	91.67	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.129		Crippen Method
mcvol	371.840	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	942.69	K	Joback Method
tc	1156.01	K	Joback Method
tf	529.40	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.74	J/mol×K	942.69	Joback Method
cpg	1239.45	J/mol×K	978.24	Joback Method
cpg	1256.82	J/mol×K	1013.80	Joback Method
cpg	1272.91	J/mol×K	1049.35	Joback Method
cpg	1287.76	J/mol×K	1084.91	Joback Method
cpg	1301.44	J/mol×K	1120.46	Joback Method
cpg	1313.99	J/mol×K	1156.01	Joback Method
dvisc	0.0003780	Pa×s	529.40	Joback Method

dvisc	0.0001783	Pa×s	598.28	Joback Method
dvisc	0.0000982	Pa×s	667.16	Joback Method
dvisc	0.0000605	Pa×s	736.05	Joback Method
dvisc	0.0000405	Pa×s	804.93	Joback Method
dvisc	0.0000289	Pa×s	873.81	Joback Method
dvisc	0.0000216	Pa×s	942.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348314&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