

Fumaric acid, 10-chlorodecyl hexyl ester

Inchi:	InChI=1S/C20H35ClO4/c1-2-3-4-12-17-24-19(22)14-15-20(23)25-18-13-10-8-6-5-7-9-11
InchiKey:	LZFDJKVRRLCZMI-CCEZHUSRSA-N
Formula:	C20H35ClO4
SMILES:	CCCCCOC(=O)C=CC(=O)OCCCCCCCCCCI
Mol. weight [g/mol]:	374.94

Physical Properties

Property code	Value	Unit	Source
gf	-282.03	kJ/mol	Joback Method
hf	-844.25	kJ/mol	Joback Method
hfus	57.53	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.569		Crippen Method
mvol	315.480	ml/mol	McGowan Method
pc	1088.50	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	851.17	K	Joback Method
tc	1044.01	K	Joback Method
tf	484.32	K	Joback Method
vc	1.232	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.51	J/molxK	851.17	Joback Method
cpg	991.30	J/molxK	883.31	Joback Method
cpg	1007.07	J/molxK	915.45	Joback Method
cpg	1021.84	J/molxK	947.59	Joback Method
cpg	1035.65	J/molxK	979.73	Joback Method
cpg	1048.52	J/molxK	1011.87	Joback Method
cpg	1060.50	J/molxK	1044.01	Joback Method
dvisc	0.0006147	Paxs	484.32	Joback Method

dvisc	0.0003015	Paxs	545.46	Joback Method
dvisc	0.0001707	Paxs	606.60	Joback Method
dvisc	0.0001073	Paxs	667.75	Joback Method
dvisc	0.0000729	Paxs	728.89	Joback Method
dvisc	0.0000526	Paxs	790.03	Joback Method
dvisc	0.0000397	Paxs	851.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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