Fumaric acid, 2,4,4-trimethylpentyl 8-chlorooctyl ester

Inchi: InChI=1S/C20H35ClO4/c1-17(15-20(2,3)4)16-25-19(23)12-11-18(22)24-14-10-8-6-5-7-9-

InchiKey: YCGNJPLNGBLDBL-VAWYXSNFSA-N

Formula: C20H35ClO4

SMILES: CC(COC(=O)C=CC(=O)OCCCCCCCCCCl)CC(C)(C)C

Mol. weight [g/mol]: 374.94

Physical Properties

Property code	Value	Unit	Source
gf	-281.63	kJ/mol	Joback Method
hf	-858.28	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	81.08	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.281		Crippen Method
mcvol	315.480	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	847.50	K	Joback Method
tc	1043.50	K	Joback Method
tf	471.74	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.80	J/mol×K	847.50	Joback Method
cpg	992.64	J/mol×K	880.17	Joback Method
cpg	1008.43	J/mol×K	912.83	Joback Method
cpg	1023.24	J/mol×K	945.50	Joback Method
cpg	1037.11	J/mol×K	978.17	Joback Method
cpg	1050.09	J/mol×K	1010.84	Joback Method
cpg	1062.22	J/mol×K	1043.50	Joback Method
dvisc	0.0006736	Pa×s	471.74	Joback Method

dvisc	0.0002926	Pa×s	534.37	Joback Method
dvisc	0.0001514	Pa×s	596.99	Joback Method
dvisc	0.0000888	Pa×s	659.62	Joback Method
dvisc	0.0000571	Pa×s	722.25	Joback Method
dvisc	0.0000394	Pa×s	784.87	Joback Method
dvisc	0.0000287	Pa×s	847.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405612&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

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