Fumaric acid, naphth-1-yl 8-chlorooctyl ester

Inchi: InChI=1S/C22H25ClO4/c23-16-7-3-1-2-4-8-17-26-21(24)14-15-22(25)27-20-13-9-11-18-1
InchiKey: CMWUKCGKDORCPR-CCEZHUSRSA-N
Formula: C22H25ClO4
SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)OCCCCCCCCCCl
Mol. weight [g/mol]: 388.88

Physical Properties

Property code	Value	Unit	Source
gf	-55.76	kJ/mol	Joback Method
hf	-469.40	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.424		Crippen Method
mcvol	300.440	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	947.57	K	Joback Method
tc	1170.47	K	Joback Method
tf	578.50	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.83	J/mol×K	947.57	Joback Method
cpg	929.41	J/mol×K	984.72	Joback Method
cpg	942.03	J/mol×K	1021.87	Joback Method
cpg	953.77	J/mol×K	1059.02	Joback Method
cpg	964.71	J/mol×K	1096.17	Joback Method
cpg	974.93	J/mol×K	1133.32	Joback Method
cpg	984.51	J/mol×K	1170.47	Joback Method
dvisc	0.0004628	Pa×s	578.50	Joback Method

dvisc	0.0002835	Pa×s	640.01	Joback Method
dvisc	0.0001892	Pa×s	701.52	Joback Method
dvisc	0.0001348	Pa×s	763.03	Joback Method
dvisc	0.0001010	Pa×s	824.55	Joback Method
dvisc	0.0000788	Pa×s	886.06	Joback Method
dvisc	0.0000635	Pa×s	947.57	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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