Fumaric acid, 4-chlorobenzyl 2-ethylhexyl ester

Inchi: InChI=1S/C19H25ClO4/c1-3-5-6-15(4-2)13-23-18(21)11-12-19(22)24-14-16-7-9-17(20)10

InchiKey: BIDFCDNQKMJUNC-VAWYXSNFSA-N

Formula: C19H25ClO4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-190.11	kJ/mol	Joback Method
hf	-603.83	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	83.09	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.699		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	859.51	K	Joback Method
tc	1070.28	K	Joback Method
tf	496.99	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.88	J/mol×K	859.51	Joback Method
cpg	834.30	J/mol×K	894.64	Joback Method
cpg	847.65	J/mol×K	929.77	Joback Method
cpg	859.96	J/mol×K	964.89	Joback Method
cpg	871.26	J/mol×K	1000.02	Joback Method
cpg	881.61	J/mol×K	1035.15	Joback Method
cpg	891.02	J/mol×K	1070.28	Joback Method
dvisc	0.0005579	Pa×s	496.99	Joback Method

dvisc	0.0002898	Pa×s	557.41	Joback Method
dvisc	0.0001711	Pa×s	617.83	Joback Method
dvisc	0.0001109	Pa×s	678.25	Joback Method
dvisc	0.0000772	Pa×s	738.67	Joback Method
dvisc	0.0000568	Pa×s	799.09	Joback Method
dvisc	0.0000436	Pa×s	859.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405919&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