Fumaric acid, monoamide, N-(4-chlorophenyl)-, 2-ethylhexyl ester

Inchi: InChI=1S/C18H24ClNO3/c1-3-5-6-14(4-2)13-23-18(22)12-11-17(21)20-16-9-7-15(19)8-1

InchiKey: MYIGZTONFLPUEF-VAWYXSNFSA-N

Formula: C18H24ClNO3

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 337.84

Physical Properties

Property code	Value	Unit	Source
gf	-4.14	kJ/mol	Joback Method
hf	-397.50	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.594		Crippen Method
mcvol	267.650	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	864.38	K	Joback Method
tc	1078.35	K	Joback Method
tf	516.15	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.41	J/mol×K	864.38	Joback Method
cpg	804.30	J/mol×K	900.04	Joback Method
cpg	817.18	J/mol×K	935.70	Joback Method
cpg	829.12	J/mol×K	971.36	Joback Method
cpg	840.16	J/mol×K	1007.02	Joback Method
cpg	850.36	J/mol×K	1042.69	Joback Method
cpg	859.76	J/mol×K	1078.35	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=U357509&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
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