Fumaric acid, 4-cyanophenyl 2-ethylhexyl ester

Inchi: InChI=1S/C19H23NO4/c1-3-5-6-15(4-2)14-23-18(21)11-12-19(22)24-17-9-7-16(13-20)8-
InchiKey: WMOIYLCWNVVWBQ-VAWYXSNFSA-N
Formula: C19H23NO4
SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 329.39

Physical Properties

Property code	Value	Unit	Source
gf	-45.00	kJ/mol	Joback Method
hf	-423.21	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.779		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	924.16	K	Joback Method
tc	1144.62	K	Joback Method
tf	532.06	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.98	J/mol×K	924.16	Joback Method
cpg	827.42	J/mol×K	960.90	Joback Method
cpg	838.77	J/mol×K	997.65	Joback Method
cpg	849.09	J/mol×K	1034.39	Joback Method
cpg	858.39	J/mol×K	1071.13	Joback Method
cpg	866.74	J/mol×K	1107.87	Joback Method
cpg	874.15	J/mol×K	1144.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405731&Units=SI

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