Fumaric acid, dec-4-enyl isohexyl ester

Inchi: InChI=1S/C20H34O4/c1-4-5-6-7-8-9-10-11-16-23-19(21)14-15-20(22)24-17-12-13-18(2)3
InchiKey: INEJRGMUNCASRS-IDRAWEHWSA-N
Formula: C20H34O4
SMILES: CCCCCC=CCCCOC(=O)C=CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-192.32	kJ/mol	Joback Method
hf	-716.57	kJ/mol	Joback Method
hfus	50.01	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.982		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	817.46	K	Joback Method
tc	1007.48	K	Joback Method
tf	434.32	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.85	J/mol×K	817.46	Joback Method
cpg	995.74	J/mol×K	975.81	Joback Method
cpg	982.15	J/mol×K	944.14	Joback Method
cpg	967.70	J/mol×K	912.47	Joback Method
cpg	952.36	J/mol×K	880.80	Joback Method
cpg	936.09	J/mol×K	849.13	Joback Method
cpg	1008.50	J/mol×K	1007.48	Joback Method
dvisc	0.0000370	Pa×s	817.46	Joback Method

dvisc	0.0000501	Pa×s	753.60	Joback Method
dvisc	0.0000717	Pa×s	689.75	Joback Method
dvisc	0.0001104	Pa×s	625.89	Joback Method
dvisc	0.0001876	Pa×s	562.03	Joback Method
dvisc	0.0003652	Pa×s	498.18	Joback Method
dvisc	0.0008646	Pa×s	434.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348940&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