Fumaric acid, pent-4-en-2-yl undecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-184.70	kJ/mol	Joback Method
hf	-708.36	kJ/mol	Joback Method
hfus	48.53	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.124		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	809.98	K	Joback Method
tc	997.70	K	Joback Method
tf	437.64	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.42	J/mol×K	809.98	Joback Method
cpg	934.66	J/mol×K	841.27	Joback Method
cpg	950.92	J/mol×K	872.55	Joback Method
cpg	966.23	J/mol×K	903.84	Joback Method
cpg	980.62	J/mol×K	935.12	Joback Method
cpg	994.11	J/mol×K	966.41	Joback Method
cpg	1006.73	J/mol×K	997.70	Joback Method
dvisc	0.0009342	Pa×s	437.64	Joback Method

dvisc	0.0004127	Pa×s	499.70	Joback Method
dvisc	0.0002184	Pa×s	561.75	Joback Method
dvisc	0.0001312	Pa×s	623.81	Joback Method
dvisc	0.0000864	Pa×s	685.87	Joback Method
dvisc	0.0000610	Pa×s	747.92	Joback Method
dvisc	0.0000454	Pa×s	809.98	Joback Method

Sources

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=U348930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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