Fumaric acid, cis-hex-3-enyl pentadecyl ester

Inchi: InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-23-29-25(27)21-20-24(26)
InchiKey: QVFWFVMMAAFYLT-VULJOHOCSA-N
Formula: C25H44O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-147.78	kJ/mol	Joback Method
hf	-814.49	kJ/mol	Joback Method
hfus	66.48	kJ/mol	Joback Method
hvap	89.47	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	853.96	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	932.30	K	Joback Method
tc	1142.51	K	Joback Method
tf	505.67	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.29	J/mol×K	932.30	Joback Method
cpg	1245.86	J/mol×K	967.33	Joback Method
cpg	1264.18	J/mol×K	1002.37	Joback Method
cpg	1281.31	J/mol×K	1037.40	Joback Method
cpg	1297.32	J/mol×K	1072.44	Joback Method
cpg	1312.29	J/mol×K	1107.47	Joback Method
cpg	1326.26	J/mol×K	1142.51	Joback Method
dvisc	0.0004022	Pa×s	505.67	Joback Method

dvisc	0.0001776	Pa×s	576.77	Joback Method
dvisc	0.0000938	Pa×s	647.88	Joback Method
dvisc	0.0000562	Pa×s	718.99	Joback Method
dvisc	0.0000370	Pa×s	790.09	Joback Method
dvisc	0.0000260	Pa×s	861.20	Joback Method
dvisc	0.0000193	Pa×s	932.30	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=U348870&Units=SI

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