Fumaric acid, hexadecyl 2-methylpentyl ester

Inchi: InChI=1S/C26H48O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-22-29-25(27)20-21-26(2
InchiKey: QPBDGPJSTQEQOR-QZQOTICOSA-N
Formula: C26H48O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-222.02	kJ/mol	Joback Method
hf	-957.63	kJ/mol	Joback Method
hfus	65.35	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.546		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	788.16	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	950.58	K	Joback Method
tc	1167.61	K	Joback Method
tf	507.02	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.93	J/mol×K	950.58	Joback Method
cpg	1338.52	J/mol×K	986.75	Joback Method
cpg	1357.62	J/mol×K	1022.92	Joback Method
cpg	1375.27	J/mol×K	1059.10	Joback Method
cpg	1391.54	J/mol×K	1095.27	Joback Method
cpg	1406.49	J/mol×K	1131.44	Joback Method
cpg	1420.19	J/mol×K	1167.61	Joback Method
dvisc	0.0004362	Pa×s	507.02	Joback Method

dvisc	0.0001808	Pa×s	580.95	Joback Method
dvisc	0.0000914	Pa×s	654.87	Joback Method
dvisc	0.0000531	Pa×s	728.80	Joback Method
dvisc	0.0000341	Pa×s	802.73	Joback Method
dvisc	0.0000236	Pa×s	876.65	Joback Method
dvisc	0.0000173	Pa×s	950.58	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=U348734&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