Fumaric acid, 2,4-dimethylpent-3-yl dodecyl ester

Inchi: InChI=1S/C23H42O4/c1-6-7-8-9-10-11-12-13-14-15-18-26-21(24)16-17-22(25)27-23(19(

InchiKey: NFBDXHSNOZVHAM-WUKNDPDISA-N

Formula: C23H42O4

SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-252.16	kJ/mol	Joback Method
hf	-906.27	kJ/mol	Joback Method
hfus	50.53	kJ/mol	Joback Method
hvap	83.90	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.231		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	881.06	K	Joback Method
tc	1079.17	K	Joback Method
tf	443.21	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.21	J/mol×K	881.06	Joback Method
cpg	1212.30	J/mol×K	1046.15	Joback Method
cpg	1197.99	J/mol×K	1013.13	Joback Method
cpg	1182.57	J/mol×K	980.11	Joback Method
cpg	1165.99	J/mol×K	947.10	Joback Method
cpg	1148.21	J/mol×K	914.08	Joback Method
cpg	1225.53	J/mol×K	1079.17	Joback Method
dvisc	0.0000229	Pa×s	881.06	Joback Method

dvisc	0.0000321	Pa×s	808.08	Joback Method
dvisc	0.0000481	Pa×s	735.11	Joback Method
dvisc	0.0000790	Pa×s	662.13	Joback Method
dvisc	0.0001465	Pa×s	589.16	Joback Method
dvisc	0.0003235	Pa×s	516.19	Joback Method
dvisc	0.0009275	Pa×s	443.21	Joback Method

Sources

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=U348553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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