Fumaric acid, hexadecyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C24H42O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-28-23(26)18-19-24(27
InchiKey: JLEVUPAWXSFZRR-VHEBQXMUSA-N
Formula: C24H42O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 410.59

Physical Properties

Property code	Value	Unit	Source
gf	-367.78	kJ/mol	Joback Method
hf	-1028.93	kJ/mol	Joback Method
hfus	61.77	kJ/mol	Joback Method
hvap	93.65	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.088		Crippen Method
mcvol	361.170	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook
tb	958.69	K	Joback Method
tc	1175.28	K	Joback Method
tf	534.41	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.11	J/mol×K	958.69	Joback Method
cpg	1287.27	J/mol×K	1139.18	Joback Method
cpg	1274.65	J/mol×K	1103.08	Joback Method
cpg	1260.77	J/mol×K	1066.99	Joback Method
cpg	1245.59	J/mol×K	1030.89	Joback Method
cpg	1229.05	J/mol×K	994.79	Joback Method
cpg	1298.70	J/mol×K	1175.28	Joback Method
dvisc	0.0000220	Pa×s	958.69	Joback Method

dvisc	0.0000296	Pa×s	887.98	Joback Method
dvisc	0.0000419	Pa×s	817.26	Joback Method
dvisc	0.0000633	Pa×s	746.55	Joback Method
dvisc	0.0001044	Pa×s	675.84	Joback Method
dvisc	0.0001934	Pa×s	605.12	Joback Method
dvisc	0.0004220	Pa×s	534.41	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=U348830&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