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

Inchi: InChI=1S/C26H46O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-30-25(28)20-21
InchiKey: LGYJKGMBWGNAES-QZQOTICOSA-N
Formula: C26H46O5
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 438.64

Physical Properties

Property code	Value	Unit	Source
gf	-350.94	kJ/mol	Joback Method
hf	-1070.21	kJ/mol	Joback Method
hfus	66.95	kJ/mol	Joback Method
hvap	98.10	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.868		Crippen Method
mcvol	389.350	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	1004.45	K	Joback Method
tc	1237.34	K	Joback Method
tf	556.95	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.99	J/mol×K	1004.45	Joback Method
cpg	1416.04	J/mol×K	1198.53	Joback Method
cpg	1403.24	J/mol×K	1159.71	Joback Method
cpg	1389.00	J/mol×K	1120.90	Joback Method
cpg	1373.27	J/mol×K	1082.08	Joback Method
cpg	1355.95	J/mol×K	1043.27	Joback Method
cpg	1427.49	J/mol×K	1237.34	Joback Method
dvisc	0.0000161	Pa×s	1004.45	Joback Method

dvisc	0.0000217	Pa×s	929.87	Joback Method
dvisc	0.0000308	Pa×s	855.28	Joback Method
dvisc	0.0000469	Pa×s	780.70	Joback Method
dvisc	0.0000780	Pa×s	706.12	Joback Method
dvisc	0.0001462	Pa×s	631.53	Joback Method
dvisc	0.0003241	Pa×s	556.95	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=U348832&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