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

Inchi: InChI=1S/C22H38O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-26-21(24)16-17-22(25)27-20
InchiKey: ZSXOHSCBRWJVHI-WUKNDPDISA-N
Formula: C22H38O5
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 382.53

Physical Properties

Property code	Value	Unit	Source
gf	-384.62	kJ/mol	Joback Method
hf	-987.65	kJ/mol	Joback Method
hfus	56.59	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.308		Crippen Method
mcvol	332.990	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		NIST Webbook
tb	912.93	K	Joback Method
tc	1117.71	K	Joback Method
tf	511.87	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.19	J/mol×K	912.93	Joback Method
cpg	1160.71	J/mol×K	1083.58	Joback Method
cpg	1148.30	J/mol×K	1049.45	Joback Method
cpg	1134.78	J/mol×K	1015.32	Joback Method
cpg	1120.12	J/mol×K	981.19	Joback Method
cpg	1104.27	J/mol×K	947.06	Joback Method
cpg	1172.05	J/mol×K	1117.71	Joback Method
dvisc	0.0000299	Pa×s	912.93	Joback Method

dvisc	0.0000401	Pa×s	846.09	Joback Method
dvisc	0.0000564	Pa×s	779.24	Joback Method
dvisc	0.0000848	Pa×s	712.40	Joback Method
dvisc	0.0001386	Pa×s	645.56	Joback Method
dvisc	0.0002536	Pa×s	578.71	Joback Method
dvisc	0.0005436	Pa×s	511.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348828&Units=SI
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

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