Fumaric acid, heptadecyl trans-hex-3-enyl ester

Inchi: InChI=1S/C27H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-21-25-31-27(29)23-22-

InchiKey: WUNDBFSYURGPIV-FHKQEHFBSA-N

Formula: C27H48O4

SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-130.94	kJ/mol	Joback Method
hf	-855.77	kJ/mol	Joback Method
hfus	71.66	kJ/mol	Joback Method
hvap	93.92	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.857		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1203.84	K	Joback Method
tf	528.21	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.80	J/mol×K	978.06	Joback Method
cpg	1374.69	J/mol×K	1015.69	Joback Method
cpg	1394.13	J/mol×K	1053.32	Joback Method
cpg	1412.23	J/mol×K	1090.95	Joback Method
cpg	1429.06	J/mol×K	1128.58	Joback Method
cpg	1444.72	J/mol×K	1166.21	Joback Method
cpg	1459.30	J/mol×K	1203.84	Joback Method
dvisc	0.0003108	Pa×s	528.21	Joback Method

dvisc	0.0001350	Pa×s	603.19	Joback Method
dvisc	0.0000706	Pa×s	678.16	Joback Method
dvisc	0.0000419	Pa×s	753.13	Joback Method
dvisc	0.0000274	Pa×s	828.11	Joback Method
dvisc	0.0000192	Pa×s	903.09	Joback Method
dvisc	0.0000142	Pa×s	978.06	Joback Method

Sources

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=U348897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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