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

Inchi: InChI=1S/C28H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-31-26(29)21-22-

InchiKey: OTDFXGNVPWSINA-QURGRASLSA-N

Formula: C28H52O4

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

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-210.06	kJ/mol	Joback Method
hf	-1009.47	kJ/mol	Joback Method
hfus	63.48	kJ/mol	Joback Method
hvap	95.03	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	8.181		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	3026.00		NIST Webbook
tb	995.46	K	Joback Method
tc	1227.17	K	Joback Method
tf	499.56	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1447.33	J/mol×K	995.46	Joback Method
cpg	1468.77	J/mol×K	1034.08	Joback Method
cpg	1488.46	J/mol×K	1072.70	Joback Method
cpg	1506.48	J/mol×K	1111.32	Joback Method
cpg	1522.90	J/mol×K	1149.94	Joback Method
cpg	1537.82	J/mol×K	1188.55	Joback Method
cpg	1551.32	J/mol×K	1227.17	Joback Method
dvisc	0.0004493	Pa×s	499.56	Joback Method
dvisc	0.0001538	Pa×s	582.21	Joback Method

dvisc	0.0000687	Pa×s	664.86	Joback Method
dvisc	0.0000367	Pa×s	747.51	Joback Method
dvisc	0.0000222	Pa×s	830.16	Joback Method
dvisc	0.0000147	Pa×s	912.81	Joback Method
dvisc	0.0000104	Pa×s	995.46	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=U348558&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