Fumaric acid, 2-heptyl hexadecyl ester

Inchi: InChI=1S/C27H50O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-20-24-30-26(28)22-23-27(
InchiKey: QQEWRVPTEKWBSJ-GHVJWSGMSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-213.60	kJ/mol	Joback Method
hf	-978.27	kJ/mol	Joback Method
hfus	67.94	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.079		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	747.33	kPa	Joback Method
rinpol	2995.00		NIST Webbook
rinpol	2995.00		NIST Webbook
tb	973.46	K	Joback Method
tc	1199.13	K	Joback Method
tf	518.29	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.13	J/mol×K	973.46	Joback Method
cpg	1472.65	J/mol×K	1161.52	Joback Method
cpg	1457.52	J/mol×K	1123.90	Joback Method
cpg	1440.98	J/mol×K	1086.29	Joback Method
cpg	1422.94	J/mol×K	1048.68	Joback Method
cpg	1403.35	J/mol×K	1011.07	Joback Method
cpg	1486.45	J/mol×K	1199.13	Joback Method
dvisc	0.0000148	Pa×s	973.46	Joback Method

dvisc	0.0000202	Pa×s	897.60	Joback Method
dvisc	0.0000292	Pa×s	821.74	Joback Method
dvisc	0.0000457	Pa×s	745.88	Joback Method
dvisc	0.0000789	Pa×s	670.01	Joback Method
dvisc	0.0001568	Pa×s	594.15	Joback Method
dvisc	0.0003810	Pa×s	518.29	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=U348633&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

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