

Fumaric acid, heptadecyl 2-hexyl ester

Inchi:	InChI=1S/C27H50O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-24-30-26(28)22-23-
InchiKey:	IRUFJGLMQRYTQT-GHVJWSGMSA-N
Formula:	C27H50O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCC
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
rinqol	2998.00		NIST Webbook
tb	973.46	K	Joback Method
tc	1199.13	K	Joback Method
tf	518.29	K	Joback Method
vc	1.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.13	J/molxK	973.46	Joback Method
cpg	1472.65	J/molxK	1161.52	Joback Method
cpg	1457.52	J/molxK	1123.90	Joback Method
cpg	1440.98	J/molxK	1086.29	Joback Method
cpg	1422.94	J/molxK	1048.68	Joback Method
cpg	1403.35	J/molxK	1011.07	Joback Method
cpg	1486.45	J/molxK	1199.13	Joback Method
dvisc	0.0000148	Paxs	973.46	Joback Method
dvisc	0.0000202	Paxs	897.60	Joback Method

dvisc	0.0000292	Paxs	821.74	Joback Method
dvisc	0.0000457	Paxs	745.88	Joback Method
dvisc	0.0000789	Paxs	670.01	Joback Method
dvisc	0.0001568	Paxs	594.15	Joback Method
dvisc	0.0003810	Paxs	518.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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