

Fumaric acid, heptadecyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C27H50O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-30-26(28)21-22-
InchiKey:	JAYQDMBLWISRTJ-QURGRASLSA-N
Formula:	C27H50O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	438.68

Physical Properties

Property code	Value	Unit	Source
gf	-216.04	kJ/mol	Joback Method
hf	-983.55	kJ/mol	Joback Method
hfus	64.42	kJ/mol	Joback Method
hvap	93.19	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.935		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	750.61	kPa	Joback Method
rinpol	2962.00		NIST Webbook
tb	973.02	K	Joback Method
tc	1197.14	K	Joback Method
tf	503.29	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.46	J/molxK	973.02	Joback Method
cpg	1472.09	J/molxK	1159.79	Joback Method
cpg	1457.13	J/molxK	1122.43	Joback Method
cpg	1440.75	J/molxK	1085.08	Joback Method
cpg	1422.90	J/molxK	1047.73	Joback Method
cpg	1403.49	J/molxK	1010.37	Joback Method
cpg	1485.71	J/molxK	1197.14	Joback Method
dvisc	0.0000134	Paxs	973.02	Joback Method
dvisc	0.0000187	Paxs	894.73	Joback Method

dvisc	0.0000276	Paxs	816.44	Joback Method
dvisc	0.0000442	Paxs	738.15	Joback Method
dvisc	0.0000794	Paxs	659.87	Joback Method
dvisc	0.0001669	Paxs	581.58	Joback Method
dvisc	0.0004419	Paxs	503.29	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=U348773&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

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