

Fumaric acid, 4-methylpent-2-yl tridecyl ester

Inchi:	InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-12-13-14-15-18-26-22(24)16-17-23(25)27-21(4)
InchiKey:	BJNVZBWSZUWQQO-WUKNDPDISA-N
Formula:	C23H42O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-249.72	kJ/mol	Joback Method
hf	-900.99	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.375		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	937.49	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	881.50	K	Joback Method
tc	1079.40	K	Joback Method
tf	458.21	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.76	J/molxK	881.50	Joback Method
cpg	1147.77	J/molxK	914.48	Joback Method
cpg	1165.55	J/molxK	947.47	Joback Method
cpg	1182.15	J/molxK	980.45	Joback Method
cpg	1197.61	J/molxK	1013.43	Joback Method
cpg	1211.97	J/molxK	1046.42	Joback Method
cpg	1225.26	J/molxK	1079.40	Joback Method
dvisc	0.0007651	Paxs	458.21	Joback Method

dvisc	0.0002957	Paxs	528.76	Joback Method
dvisc	0.0001430	Paxs	599.31	Joback Method
dvisc	0.0000806	Paxs	669.86	Joback Method
dvisc	0.0000506	Paxs	740.40	Joback Method
dvisc	0.0000345	Paxs	810.95	Joback Method
dvisc	0.0000250	Paxs	881.50	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=U348327&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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