

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

Inchi:	InChI=1S/C14H24O4/c1-6-9-17-12(15)7-8-13(16)18-14(10(2)3)11(4)5/h7-8,10-11,14H,6,
InchiKey:	AIBLZADNUJSYBQ-BQYQJAHWSA-N
Formula:	C14H24O4
SMILES:	CCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-327.94	kJ/mol	Joback Method
hf	-720.51	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.720		Crippen Method
mvol	218.700	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1616.00		NIST Webbook
tb	675.14	K	Joback Method
tc	864.61	K	Joback Method
tf	341.78	K	Joback Method
vc	0.830	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.55	J/molxK	675.14	Joback Method
cpg	673.06	J/molxK	833.03	Joback Method
cpg	660.36	J/molxK	801.46	Joback Method
cpg	646.87	J/molxK	769.88	Joback Method
cpg	632.58	J/molxK	738.30	Joback Method
cpg	617.48	J/molxK	706.72	Joback Method
cpg	684.98	J/molxK	864.61	Joback Method
dvisc	0.0000821	Paxs	675.14	Joback Method
dvisc	0.0001138	Paxs	619.58	Joback Method

dvisc	0.0001681	Paxs	564.02	Joback Method
dvisc	0.0002705	Paxs	508.46	Joback Method
dvisc	0.0004891	Paxs	452.90	Joback Method
dvisc	0.0010436	Paxs	397.34	Joback Method
dvisc	0.0028493	Paxs	341.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348542&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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