

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

Inchi:	InChI=1S/C18H32O4/c1-5-7-8-9-10-11-14-21-17(19)12-13-18(20)22-16(6-2)15(3)4/h12-1
InchiKey:	DGNUMEHPOGGUVFD-OUKQBFOZSA-N
Formula:	C18H32O4
SMILES:	CCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-291.82	kJ/mol	Joback Method
hf	-797.79	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.424		Crippen Method
mvol	275.060	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	767.10	K	Joback Method
tc	952.42	K	Joback Method
tf	401.86	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.20	J/molxK	767.10	Joback Method
cpg	843.39	J/molxK	797.99	Joback Method
cpg	859.63	J/molxK	828.87	Joback Method
cpg	874.95	J/molxK	859.76	Joback Method
cpg	889.37	J/molxK	890.65	Joback Method
cpg	902.91	J/molxK	921.53	Joback Method
cpg	915.59	J/molxK	952.42	Joback Method
dvisc	0.0014223	Paxs	401.86	Joback Method

dvisc	0.0005699	Paxs	462.73	Joback Method
dvisc	0.0002825	Paxs	523.61	Joback Method
dvisc	0.0001620	Paxs	584.48	Joback Method
dvisc	0.0001032	Paxs	645.35	Joback Method
dvisc	0.0000711	Paxs	706.23	Joback Method
dvisc	0.0000519	Paxs	767.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348765&Units=SI

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
mccvol:	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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