

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

Inchi: InChI=1S/C19H34O4/c1-5-7-8-9-10-11-12-15-22-18(20)13-14-19(21)23-17(6-2)16(3)4/h1-4,11-14,16-18,20-21,23-24H
InchiKey: IYUMQZAITASHJI-BUHFOSPRSA-N
Formula: C19H34O4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.40	kJ/mol	Joback Method
hf	-818.43	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.814		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinqol	2168.00		NIST Webbook
tb	789.98	K	Joback Method
tc	976.37	K	Joback Method
tf	413.13	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.08	J/molxK	789.98	Joback Method
cpg	902.61	J/molxK	821.05	Joback Method
cpg	919.15	J/molxK	852.11	Joback Method
cpg	934.72	J/molxK	883.18	Joback Method
cpg	949.36	J/molxK	914.24	Joback Method
cpg	963.08	J/molxK	945.31	Joback Method
cpg	975.91	J/molxK	976.37	Joback Method
dvisc	0.0012655	Paxs	413.13	Joback Method
dvisc	0.0005031	Paxs	475.94	Joback Method

dvisc	0.0002480	Paxs	538.75	Joback Method
dvisc	0.0001417	Paxs	601.56	Joback Method
dvisc	0.0000900	Paxs	664.36	Joback Method
dvisc	0.0000618	Paxs	727.17	Joback Method
dvisc	0.0000451	Paxs	789.98	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=U348766&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
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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