

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

Inchi:	InChI=1S/C29H54O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-32-27(30)22-
InchiKey:	DVTMOXKNWRFYKI-GHVJWSGMSA-N
Formula:	C29H54O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	466.74

Physical Properties

Property code	Value	Unit	Source
gf	-201.64	kJ/mol	Joback Method
hf	-1030.11	kJ/mol	Joback Method
hfus	66.07	kJ/mol	Joback Method
hvap	97.25	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	8.571		Crippen Method
mvol	430.050	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	3128.00		NIST Webbook
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tb	1018.34	K	Joback Method
tc	1260.34	K	Joback Method
tf	510.83	K	Joback Method
vc	1.669	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1512.24	J/molxK	1018.34	Joback Method
cpg	1604.55	J/molxK	1220.01	Joback Method
cpg	1589.51	J/molxK	1179.67	Joback Method
cpg	1572.86	J/molxK	1139.34	Joback Method
cpg	1554.50	J/molxK	1099.01	Joback Method
cpg	1534.32	J/molxK	1058.67	Joback Method
cpg	1618.08	J/molxK	1260.34	Joback Method
dvisc	0.0000089	Paxs	1018.34	Joback Method

dvisc	0.0000125	Paxs	933.75	Joback Method
dvisc	0.0000189	Paxs	849.17	Joback Method
dvisc	0.0000313	Paxs	764.59	Joback Method
dvisc	0.0000588	Paxs	680.00	Joback Method
dvisc	0.0001318	Paxs	595.42	Joback Method
dvisc	0.0003864	Paxs	510.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348559&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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