

Fumaric acid, eicosyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C29H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-32-28(3)
InchiKey: LGWZJUAPFJXRPL-WCWDXBQESA-N
Formula: C29H54O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-199.20	kJ/mol	Joback Method
hf	-1024.83	kJ/mol	Joback Method
hfus	69.60	kJ/mol	Joback Method
hvap	97.64	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	8.715		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	677.46	kPa	Joback Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		NIST Webbook
tb	1018.78	K	Joback Method
tc	1263.11	K	Joback Method
tf	525.83	K	Joback Method
vc	1.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.99	J/molxK	1018.78	Joback Method
cpg	1605.53	J/molxK	1222.39	Joback Method
cpg	1590.27	J/molxK	1181.67	Joback Method
cpg	1573.39	J/molxK	1140.94	Joback Method
cpg	1554.79	J/molxK	1100.22	Joback Method
cpg	1534.35	J/molxK	1059.50	Joback Method
cpg	1619.27	J/molxK	1263.11	Joback Method
dvisc	0.0000098	Paxs	1018.78	Joback Method

dvisc	0.0000136	Paxs	936.62	Joback Method
dvisc	0.0000201	Paxs	854.46	Joback Method
dvisc	0.0000324	Paxs	772.31	Joback Method
dvisc	0.0000585	Paxs	690.15	Joback Method
dvisc	0.0001238	Paxs	607.99	Joback Method
dvisc	0.0003313	Paxs	525.83	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=U348091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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