

Fumaric acid, eicosyl 3-methylbut-3-enyl ester

Inchi:

InChI=1S/C29H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-32-28(30

InchiKey:

QDXQGVXPSLCVJV-GHVJWSGMSA-N

Formula:

C29H52O4

SMILES:

C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]:

464.72

Physical Properties

Property code	Value	Unit	Source
gf	-115.03	kJ/mol	Joback Method
hf	-898.63	kJ/mol	Joback Method
hfus	74.05	kJ/mol	Joback Method
hvap	97.83	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.637		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	688.53	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1016.22	K	Joback Method
tc	1259.87	K	Joback Method
tf	540.11	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.53	J/mol×K	1016.22	Joback Method
cpg	1502.72	J/mol×K	1056.83	Joback Method
cpg	1523.13	J/mol×K	1097.44	Joback Method
cpg	1541.88	J/mol×K	1138.05	Joback Method
cpg	1559.08	J/mol×K	1178.66	Joback Method
cpg	1574.82	J/mol×K	1219.26	Joback Method
cpg	1589.23	J/mol×K	1259.87	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=U348919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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