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

Inchi: InChI=1S/C20H34O4/c1-4-5-6-7-8-9-10-11-12-16-23-19(21)13-14-20(22)24-17-15-18(2)3

InchiKey: VWMDQEGIJATUJW-BUHFOSPRSA-N

Formula: C20H34O4

SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-190.81	kJ/mol	Joback Method
hf	-712.87	kJ/mol	Joback Method
hfus	50.74	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.126		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	2364.00		NIST Webbook
tb	810.30	K	Joback Method
tc	997.87	K	Joback Method
tf	438.68	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.54	J/mol×K	810.30	Joback Method
cpg	933.77	J/mol×K	841.56	Joback Method
cpg	950.03	J/mol×K	872.82	Joback Method
cpg	965.35	J/mol×K	904.08	Joback Method
cpg	979.76	J/mol×K	935.35	Joback Method
cpg	993.30	J/mol×K	966.61	Joback Method
cpg	1005.99	J/mol×K	997.87	Joback Method

Sources

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=U348910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume