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

Inchi: InChI=1S/C15H17NO6/c1-10(2)11(3)21-14(17)8-9-15(18)22-13-7-5-4-6-12(13)16(19)20/l
InchiKey: YAAUBFYQDKQPFN-CMDGGOBGSA-N
Formula: C15H17NO6
SMILES: CC(C)C(C)OC(=O)C=CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 307.30

Physical Properties

Property code	Value	Unit	Source
gf	-178.75	kJ/mol	Joback Method
hf	-521.57	kJ/mol	Joback Method
hfus	38.35	kJ/mol	Joback Method
hvap	86.01	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.644		Crippen Method
mcvol	226.450	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	881.96	K	Joback Method
tc	1117.89	K	Joback Method
tf	550.60	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.55	J/mol×K	881.96	Joback Method
cpg	683.29	J/mol×K	921.28	Joback Method
cpg	693.89	J/mol×K	960.60	Joback Method
cpg	703.37	J/mol×K	999.92	Joback Method
cpg	711.79	J/mol×K	1039.25	Joback Method
cpg	719.17	J/mol×K	1078.57	Joback Method
cpg	725.55	J/mol×K	1117.89	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=U405793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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